

Vacuum-Bounded States and the Entropy of Black Hole Evaporation

by

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Abstract

We call a state “vacuum bounded” if every measurement performed outside a specified interior region gives the same result as in the vacuum. We compute the maximum entropy of a vacuum-bounded state with a given energy for a one-dimensional model, with the aid of numerical calculations on a lattice. For large energies we show that a vacuum-bounded system with length L_{in} and a given energy has entropy no more than $S^{\text{rb}} + \frac{1}{6} \ln S^{\text{rb}}$, where S^{rb} is the entropy in a rigid box with the same size and energy. Assuming that the state resulting from the evaporation of a black hole is similar to a vacuum-bounded state, and that the similarity between vacuum-bounded and rigid box problems extends from 1 to 3 dimensions, we apply these results to the black hole information paradox. Under these assumptions we conclude that large amounts of information cannot be emitted in the final explosion of a black hole.

We also consider vacuum-bounded states at very low energies and come to the surprising conclusion that the entropy of such a state can be much higher than that of a rigid box state with the same energy. For a fixed E we let L'_{in} be the length of a rigid box which gives the same entropy as a vacuum-bounded state of length L_{in} . In the $E \rightarrow 0$ limit we conjecture that the ratio $L'_{\text{in}}/L_{\text{in}}$ grows without bound and support this conjecture with numerical computations.

Thesis Supervisor: Alan H. Guth
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To Judy and Valerie, with love.

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Notation

Symbol	Meaning	First used
a, a^\dagger	Raising and lowering operators for normal modes of H	34
A	Arbitrary operator	18
$A^{(n)}$	Sequence of operators	18
\bar{A}	Limit of $A^{(n)}$	18
b, b^\dagger	Raising and lowering operators for improved vacuum normal modes	35
C_α	General constraint operator	17
\bar{D}, \bar{D}'	Free part of outside oscillators: initial form	39
D, D'	Free part of outside oscillators: final form	38
E	Energy	18
E_0	Average energy of vacuum-bounded state	15
f, g	Coefficients of constraints in $\ln \rho$	37
$f(x)$	Coupling coefficient ratio	52
g	Effective number of degrees of freedom at T_{unk}	15
$g(x)$	Continuum eigenfunction	53
\mathcal{G}	Space of states of “ground-state” modes	36
H	Operator used to define $\mathcal{P}(E)$	18
H	Hamiltonian of original vacuum	31
\tilde{H}	Space of states of “free” modes	36
H'	Alternate Hamiltonian with same vacuum	34
H'	Fictitious Hamiltonian	37
\mathcal{H}	Hilbert space of states	17
\mathcal{H}'	Subspace of \mathcal{H} on which every admissible ρ is non-vanishing	27
K	Potential coupling matrix of vacuum	32
\tilde{K}	Potential coupling matrix of reduced vacuum	40
K'	Potential couplings in H'	42
l_{pl}	Planck energy	15
L_1	Lattice spacing	33
L_{in}	Length of inside region	31
L'_{in}	Equivalent length of system with same S and E	63
m_{pl}	Planck mass	15
M_0	Mass of black hole at cutoff	15
N_{free}	Number of “free” modes	35
N_{gs}	Number of “ground state” modes	35

N_{in}	— Number of inside oscillators	33
N_{norm}	— Number of “normal” modes	58
N_{out}	— Number of outside oscillators	33
N_{α}, N_n	— Normalization factors in normal modes	49
\mathcal{N}	— Nullspace of ρ	27
O_{out}^{α}	— Operator made of outside fields	32
$p_k(\rho)$	— The k th largest eigenvalue of ρ	23
\mathbf{P} or \mathbf{P}_x	— Momentum associated with \mathbf{x}	32
\mathbf{P}_u	— Momentum associated with \mathbf{u}	47
\mathbf{P}_w	— Momentum associated with \mathbf{w}	39
\mathbf{P}_y	— Momentum associated with \mathbf{y}	35
\mathbf{P}_z	— Momentum associated with \mathbf{z}	34
\mathbb{P}	— Matrix of pairs of position operators	33
\mathbb{P}_w	— Matrix of pairs of \mathbf{P}_w operators	40
\mathbb{P}_z	— Matrix of pairs of \mathbf{P}_z operators	34
\mathcal{P}	— Space of admissible density matrices	18
$\mathcal{P}_=(E; V_1, V_2, \dots)$	— Space of ρ satisfying equality constraints	25
$\mathcal{P}_{\leq}(E; V_1, V_2, \dots)$	— Space of ρ satisfying bounds	25
Q	— Grand partition function	30
Q	— Transformation between \mathbf{x} and \mathbf{w}	39
Q_{out}^a	— Operator quadratic in outside fields	32
R	— Radius of inside region	16
R	— Transformation between \mathbf{x}_{out} and \mathbf{w}_{out}	38
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T_{unk}	— Temperature of unknown physics	15
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\mathbb{Z}	— Matrix of pairs of \mathbf{z} operators	34

β	— Inverse temperature	30
γ	— Euler's constant	62
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$\delta A(E)$	— Difference in quantity A at same energy	69
$\delta A(T)$	— Difference in quantity A at same temperature	69
Δ	— Fraction by which equivalent rigid system is larger	65
$\pi(x)$	— Scalar field momentum	31
ρ	— Density matrix	17
$\rho^{(n)}$	— Sequence of density matrices	21
$\hat{\rho}^{(n)}$	— Cauchy subsequence of density matrix sequence	22
$\bar{\rho}$	— Limit of a sequence of density matrices	21
τ	— Temperature scaled by L_{in}	68
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¹These routines and many others are now available on a CDROM [2]

Chapter 1

Introduction

1.1 Background

Since the discovery of black hole radiation by Hawking [3], the fate of information falling into a black hole has been a mystery. (See [4–6] for reviews.) If Hawking’s semiclassical calculation is correct, then the outgoing radiation is purely thermal and the outgoing photons are uncorrelated to each other and to the matter which formed the black hole. If the evaporation is complete, and if the thermal nature of the radiation persists throughout the evaporation, then the original information is lost. Thus if the black hole is formed from a quantum-mechanically pure state, there will nevertheless be a mixed state after the evaporation is complete. This is the position held by Hawking (e.g. see [7]), but it violates CPT and may lead to difficulties with energy conservation and causality [4,8–10].

If information is not lost in black hole evaporation, there are several possibilities. One is that the black hole does not evaporate completely, but instead produces one or more Planck-scale remnants (e.g. see [6]). Another possibility is that the information disappears into a baby universe [11]. In this scenario the quantum-mechanical pure state is preserved, but parts of it are inaccessible to observation. It is also possible that the radiation is not really thermal, even at early times, because of a complementarity principle [12–15] or the inapplicability of the semiclassical approach [16–19], and thus that the information is encoded in subtle correlations in the radiation. In this case the black hole could act like a normal object with the entropy describing internal degrees of freedom. Some results from string theory [20–23] tend to confirm this view.

Even if the radiation is thermal and uncorrelated during most of the evaporation, there is no reason to believe that it remains thermal near the endpoint of the evaporation. The late-time radiation is presumably governed by an unknown theory of quantum gravity, and may well have correlations to the radiation emitted earlier.¹ However, it is generally believed that late-time radiation cannot resolve the information paradox [24,5,6]. The argument goes as follows: While the black hole is large,

¹This is conceivable because at early times information in the outgoing radiation can be correlated with information in the ingoing negative-energy flux.

it is presumably radiating high-entropy thermal radiation. If the final explosion is to restore a pure state, it must radiate as much entropy² as was radiated in earlier times. However, by the time the black hole reaches the point where unknown physics could come into play, there is little energy remaining. To radiate a lot of information with little energy requires a long period of time, and thus the “final explosion” looks more like a long-lived remnant.

However, Wilczek and Holzhey [25] argue from a moving mirror model that a state with high entropy can nevertheless be purified with arbitrarily low energy cost. In certain ways, their model looks more like a remnant theory than a complete-evaporation theory, but it still appears to cast some doubt on the standard argument above.

In any case, this argument requires bounding the entropy that can be contained in a particular region with a fixed energy. In the case of a region with reflecting walls, this is the question of finding the thermal state of quantum fields in a box. For a spherical box and a particular field theory the problem is easily solved. But with a region of complex shape, or where one wishes to make a statement intended to apply to all field theories, the situation is more complicated. Bekenstein [26,27] argues that such a universal bound exists, but Unruh and Wald [28] disagree.

Here we take a different approach. We consider only a single scalar field, but we use a weaker and, we hope, more physical condition on the results of the black hole evaporation. In the end, our results still support the claim that late-time radiation cannot restore the purity of the state of an evaporating black hole.

We will also make a more general investigation of our new definition of a localized state. In the very low energy regime we will find the surprising result that this definition gives rise to much higher entropy than the same energy could support in a rigid box. In the low-energy limit we conjecture that this difference grows without bound.

1.2 The vacuum-bounded state

1.2.1 Black hole evaporation

We start by considering a black hole formed from a pure quantum-mechanical state of incoming matter. To avoid any possible complications of quantum gravity theory, we will look at the state produced after the black hole has completely evaporated [5]. Gravity should play no significant role in this state, since the energy density should be small everywhere.³ We can describe the final state as follows: at large distances from the position of the black hole (taken as the origin) there is outgoing Hawking radiation, which we are assuming to be thermal and without internal correlations. Within some distance R of the origin, there is some state of ordinary quantum fields that could

²Here and throughout this thesis, “entropy” means fine-grained quantum-mechanical entropy.

³If instead there are Planck-scale concentrations of energy, then we would have a remnant theory, a possibility we are explicitly not considering here.

have correlations with the radiation emitted earlier. The distance R is the distance that such information might have propagated since unknown physics came into play. Let us assume that Hawking's semi-classical calculation is good up to an energy scale T_{unk} . This temperature is reached when the black hole's mass is⁴ $M_0 = 1/(8\pi T_{\text{unk}})$. If, after this, the rate of evaporation continues to match the Hawking calculation,⁵ the black hole will evaporate in time $t \sim 10^4 M_0^3/g \sim 1/(g T_{\text{unk}}^3)$, where g is the effective number of degrees of freedom in the particles that can be radiated. (See [29].) So there is a sphere of radius

$$R \sim \frac{1}{g T_{\text{unk}}^3} \quad (1.1)$$

which contains total energy

$$E_0 = \frac{1}{8\pi T_{\text{unk}}} \quad (1.2)$$

in which the information could be contained. Taking, for example, $T_{\text{unk}} = 10^{15} \text{ GeV} \sim 10^{-4} m_{\text{pl}}$, and $g \sim 100$ we get⁶

$$R \sim 10^{10} l_{\text{pl}} \sim 10^{-23} \text{ cm} \quad (1.3a)$$

$$E_0 \sim 10^3 m_{\text{pl}} \sim 10^{-2} \text{ g} \sim 10^{19} \text{ erg}. \quad (1.3b)$$

This yields a somewhat outrageous density of 10^{65} g/cm^3 , which is nevertheless small compared to the "GUT density" $(10^{16} \text{ GeV})^4/(\hbar^3 c^5) \sim 10^{81} \text{ g/cm}^3$.

1.2.2 The vacuum-bounded condition

Now we would like to answer the following question: How much entropy can be contained in a spherical region of radius R with a total energy E_0 ? To answer this question we have to specify what we mean by "contained in a region." As mentioned earlier, if we ask how much entropy can be contained in a spherical box of radius R with perfectly reflecting walls, the question can be easily answered. However, the system with the box is not so closely akin to the system under discussion. For instance, inserting the reflecting walls into the system produces a divergent increase in the ground-state energy of the system. Furthermore, if we started with the vacuum in the whole system, and then introduced a spherical wall, we would produce a divergent geometric entropy [30–33]. A better description of our system is simply that it has thermal radiation outside radius R , and an unknown state of the quantum fields inside radius R , but no barrier or boundary at R .

To study such systems, we will assume that the difference between the external Hawking radiation and an external vacuum is not important to considerations of

⁴We are working with units in which $c = G = \hbar = k_B = 1$

⁵As opposed, for example, to slowing to nothing and leaving a remnant.

⁶Another possibility is that g diverges as $T \rightarrow m_{\text{pl}}$. In this case the information can be radiated in a small number of particles of about the Planck mass, chosen from an infinite spectrum of such particles. This is effectively a remnant theory.

entropy.⁷ We will study systems that have an arbitrary state inside R but the vacuum outside R . To make this precise we will specify the problem as follows:

Let a *vacuum-bounded state* be a generalized state (i.e. density matrix) for which every operator composed of fields at points outside a specified interior region has the same expectation value as in the vacuum. What is the maximum entropy of such a state whose interior region is a sphere of radius R and whose total average energy⁸ is given by $\langle H \rangle = E_0$?

We expect to find that the answer to this question is similar to that of a box of radius R with reflecting walls, with some small correction.

We will denote by X_{in} quantities in the given interior region and by X_{out} those outside this region. We will say that a generalized state is “localized to the inside” or “obeys the vacuum-bounded condition” if any measurement performed on the outside field operators in this state yields the same result as in the vacuum, i.e. if

$$\text{Tr } \rho O_{\text{out}} = \text{Tr } \rho^{\text{vac}} O_{\text{out}} = \langle 0 | O_{\text{out}} | 0 \rangle \quad (1.4)$$

for every operator O_{out} that is constructed from field operators in the outside region.

In the language of density matrices, we can write $\rho_{\text{out}} = \text{Tr}_{\text{in}} \rho$, where ρ is the overall density matrix describing our system and Tr_{in} means to trace over all the “inside” variables. Then ρ_{out} is the reduced density matrix describing only the outside variables, and Eq. (1.4) is equivalent to

$$\rho_{\text{out}} = \rho_{\text{out}}^{\text{vac}} \equiv \text{Tr}_{\text{in}} |0\rangle\langle 0|, \quad (1.5)$$

where $|0\rangle$ denotes the ground state.

⁷If this approximation is bad we can increase R until the Hawking radiation outside R has very low temperature.

⁸We cannot specify that every measurement of the energy must give E_0 . Such a state is necessarily static and thus cannot represent outgoing radiation.

Chapter 2

Mathematical Considerations

In this chapter we will prove some theorems regarding the general theory of constrained density operators. Our goals are to show that there is always a unique operator which maximizes the entropy subject to the constraints and to demonstrate the form of that operator. Unfortunately we will not accomplish either of these goals completely, although we will make some progress in these directions. In particular we will show that if such a operator exists it is unique, and that an operator of the form specified, if one exists, does in fact maximize the entropy.

2.1 Topology of the space of density operators

Definition *Let \mathcal{H} be a separable Hilbert space, and let ρ be a linear operator on \mathcal{H} . Then ρ is a density operator (or density matrix) if and only if*

- ρ is Hermitian
- ρ is trace-class and $\text{Tr } \rho = 1$
- $\langle \psi | \rho | \psi \rangle \geq 0$ for any state $|\psi\rangle$.

The last property is usually written “ ρ is positive semidefinite” (or sometimes “positive definite”) by physicists and “ ρ is positive” or “ $\rho \geq 0$ ” by mathematicians. In this section we will usually use the latter notation.

We will require our operators ρ to satisfy a set of constraints of the form

$$\text{Tr } \rho C_\alpha = V_\alpha \tag{2.1}$$

for some given operators C_α and numbers V_α . (By $\text{Tr } A = a$ we mean that A is trace-class and its trace is a .) We would like to find the density operator ρ which maximizes the entropy $S = -\text{Tr } \rho \ln \rho$ subject to the constraints. There are two potential problems here. First, there might be states with arbitrarily large entropy. If there are no constraints, that will be the case whenever \mathcal{H} has infinite dimension. Second, there might be a supremum of the possible values of S which is not achieved by any ρ .

In an attempt to address these problems we would like to prove some continuity results for S and some compactness results for the space of allowable ρ . However, if any density operator is allowed, then those with infinite entropy or infinite energy are dense in the space of all density operators, using any reasonable norm. Thus S cannot be continuous on such a space. Instead we will work only with those ρ for which $\text{Tr } \rho H$ is bounded, where H is some reasonable Hamiltonian.

Since density operators are trace-class they are also Hilbert-Schmidt operators, and we can use the Hilbert-Schmidt inner product $(\rho, \rho') = \text{Tr } \rho \rho'$ and the corresponding norm given by $\|\rho\|_2 = \sqrt{\text{Tr } \rho^2}$. The topology on the space of operators will always be that induced by $\|\cdot\|_2$. We will write $\|\cdot\|$ for the norm of a state and for the bound on a bounded operator, and $\|\cdot\|_2$ for the Hilbert-Schmidt norm of an operator.

2.1.1 Compactness

We will first show that with an energy bound the space of density operators is compact.

Theorem 1 *Let \mathcal{H} be a separable Hilbert space, let H be a positive Hermitian operator on \mathcal{H} with a purely discrete spectrum, and suppose further that no infinite-dimensional subspace exists on which H is bounded.¹ For some $E > 0$ let $\mathcal{P}(E)$ be the space of density operators ρ on \mathcal{H} such that $\text{Tr } \rho H \leq E$. Then the space \mathcal{P} is compact in the topology induced by $\|\cdot\|_2$.*

The proof is composed of a series of lemmas.

Lemma 1 *Let $\{A_n\}$ be a sequence of operators on \mathcal{H} and suppose that $\lim_{n \rightarrow \infty} A^{(n)} = \bar{A}$. Then $\lim_{n \rightarrow \infty} A_{\alpha\beta}^{(n)} = \bar{A}_{\alpha\beta}$ where $A_{\alpha\beta}$ denotes a matrix element of A in some orthonormal basis $\{|\alpha\rangle\}$.*

Proof: If $A^{(n)} \rightarrow \bar{A}$ then $\|A^{(n)} - \bar{A}\|_2 \rightarrow 0$. We can use the basis $\{|\alpha\rangle\}$ to compute the norm,

$$\|A^{(n)} - \bar{A}\|_2 = \sum_{\alpha\beta} |\langle\alpha|A^{(n)} - \bar{A}|\beta\rangle|^2 = \sum_{\alpha\beta} |A_{\alpha\beta}^{(n)} - \bar{A}_{\alpha\beta}|^2, \quad (2.2)$$

so each $|A_{\alpha\beta}^{(n)} - \bar{A}_{\alpha\beta}| \rightarrow 0$ and thus $A_{\alpha\beta}^{(n)} \rightarrow \bar{A}_{\alpha\beta}$. ■

Lemma 2 *Let $\{A^{(n)}\}$ be a sequence of positive operators on \mathcal{H} with $A^{(n)} \rightarrow \bar{A}$. Then $\bar{A} \geq 0$.*

Proof: Let $|x'\rangle$ be any element of \mathcal{H} . Define a normalized vector $|x\rangle = |x'\rangle / \||x'\rangle\|$. We can always make a basis with $|x\rangle$ as one of its elements. From lemma 1, $A_{xx}^{(n)} \rightarrow \bar{A}_{xx}$. Thus

$$\langle x|\bar{A}|x\rangle = \lim_{n \rightarrow \infty} \langle x|A^{(n)}|x\rangle. \quad (2.3)$$

¹If such an infinite-dimensional subspace does exist then there are states with infinite entropy for any E .

Since $A^{(n)} \geq 0$ we have $\langle x|A^{(n)}|x\rangle \geq 0$ for any $|x\rangle$. Since the limit of positive numbers cannot be negative, $\langle x|\bar{A}|x\rangle \geq 0$ and thus $\langle x'|\bar{A}|x'\rangle \geq 0$ for any $|x'\rangle$. That is to say, $\bar{A} \geq 0$. ■

Lemma 3 *Let B be any positive operator on \mathcal{H} with a purely discrete spectrum. Let $\{A^{(n)}\}$ be a sequence of positive operators with $A^{(n)} \rightarrow \bar{A}$. Suppose that $\text{Tr } A^{(n)}B \leq B_0$ for all n . Then $\text{Tr } \bar{A}B \leq B_0$.*

Proof: We work in a basis where B is diagonal. We write the trace

$$\text{Tr } \bar{A}B = \lim_{N \rightarrow \infty} \sum_{n=1}^N \bar{A}_{nn} B_n. \quad (2.4)$$

For each N this is a finite sum. By lemma 1 the elements of $A^{(i)}$ converge individually to the elements of \bar{A} . Thus

$$\sum_{n=1}^N \bar{A}_{nn} B_n = \lim_{i \rightarrow \infty} \sum_{n=1}^N A_{nn}^{(i)} B_n. \quad (2.5)$$

Since $A^{(i)} \geq 0$, the diagonal elements of $A^{(i)}$ cannot be negative, and since $B \geq 0$ we have $B_n \geq 0$ for every n . Thus

$$\sum_{n=1}^N A_{nn}^{(i)} B_n \leq \text{Tr } A^{(i)} B \leq B_0. \quad (2.6)$$

By Eq. (2.6) the terms in the limit in Eq. (2.5) are each no more than B_0 , and thus

$$\sum_{n=1}^N \bar{A}_{nn} B_n \leq B_0. \quad (2.7)$$

Thus each term in the limit in Eq. (2.4) is not more than B_0 and so $\text{Tr } \bar{A}B \leq B_0$. ■

Note that lemma 3 would not hold with \leq replaced by $=$, as shown by the following counterexample: Let $B = \text{diag}(1, 2, 3, 4, \dots)$. For any n let $A^{(n)} = 0$ except for the n th diagonal element which is $1/n$. By making n large we can make $\|A^{(n)}\|_2 = 1/n$ as small as desired. Thus $A^{(n)} \rightarrow \bar{A} = 0$. However, $\text{Tr } A^{(n)}B = 1$ for all n , whereas $\text{Tr } \bar{A}B = 0$.

We will now work in a basis $\{|n\rangle\}$ where H is diagonal, $H_{mn} = \langle m|H|n\rangle = \delta_{mn}E_n$ with $E_n \leq E_{n+1}$.

Lemma 4 *Let A be any positive operator with $\text{Tr } AH \leq E$. Given any $\epsilon > 0$ there is some number N such that for every positive operator A with $\text{Tr } AH \leq E$,*

$$\sum_{n=N}^{\infty} \langle n|A|n\rangle \leq \epsilon. \quad (2.8)$$

Note that $\text{Tr } AH \leq E$ implies that A is trace-class and consequently that for any given A , there is an N with $\sum_N^\infty A_{nn} \leq \epsilon$. The point of lemma 4 is that such an N can be chosen uniformly for all A .

Proof: We have

$$\sum_{n=1}^{\infty} A_{nn} E_n = \text{Tr } AH \leq E. \quad (2.9)$$

Since $A \geq 0$ we have $A_{nn} \geq 0$ for every n . Since the E_n are increasing,

$$\sum_{n=N}^{\infty} A_{nn} E_N < \sum_{n=N}^{\infty} A_{nn} E_n \leq E \quad (2.10)$$

so

$$\sum_{n=N}^{\infty} A_{nn} < \frac{E}{E_N}. \quad (2.11)$$

Since H is unbounded on any infinite-dimensional subspace, we can find E_N arbitrarily large. Thus for any $\epsilon > 0$ we can find an N such that

$$\sum_{n=N}^{\infty} A_{nn} < \epsilon \quad (2.12)$$

for every A with $\text{Tr } AH \leq E$. ■

Lemma 5 *Given any $\epsilon > 0$ there is a $\delta > 0$ such that for any positive operators A and A' with $\text{Tr } AH \leq E$ and $\text{Tr } AH' \leq E$, if $\|A - A'\|_2 < \delta$ then $|\text{Tr}(A - A')| < \epsilon$.*

Proof: Let $\rho_{\downarrow N}$ denote the $N \times N$ matrix given by ρ_{ab} with $a, b = 1 \dots N$. By lemma 4 we can find N such that

$$\text{Tr}(A - A_{\downarrow N}) = \sum_{n=N}^{\infty} A_{nn} < \frac{\epsilon}{3} \quad (2.13)$$

for any positive operator A with $\text{Tr } AH \leq E$. Let

$$\delta = \frac{\epsilon}{3\sqrt{N}}. \quad (2.14)$$

Then for any A and A' with $\|A - A'\| < \delta$ we have

$$(\text{Tr}(A_{\downarrow N} - A'_{\downarrow N}))^2 = \left(\sum_{n=1}^N (A_{nn} - A'_{nn}) \right)^2 \leq N \sum_{a=1}^N (A_{nn} - A'_{nn})^2 \leq N \|A - A'\|_2^2 < \frac{\epsilon^2}{9}, \quad (2.15)$$

so

$$|\text{Tr}(A_{\downarrow N} - A'_{\downarrow N})| < \frac{\epsilon}{3}. \quad (2.16)$$

If $\text{Tr } AH \leq E$ and $\text{Tr } A'H \leq E$ we can add Eqs. (2.13) and (2.16) to get

$$|\text{Tr } A - \text{Tr } A'| \leq |\text{Tr } (A - A \downarrow_N)| + |\text{Tr } (A \downarrow_N - A' \downarrow_N)| + |\text{Tr } (A' \downarrow_N - A')| < \epsilon. \blacksquare \quad (2.17)$$

Lemma 6 *Let A be a trace-class operator and C be a bounded operator. Then AC is trace-class and $\text{Tr}|A|C \leq |\text{Tr } A| \times \|C\|$.*

Proof: Since A is trace-class it has a purely discrete spectrum. Thus we can write $A = \sum A_n |n\rangle \langle n|$ with $\langle n|n\rangle = 1$. By the triangle inequality, $\langle n|C|n\rangle \leq \| |n\rangle\| \times \|C|n\rangle\| \leq \|C\|$. Then

$$\text{Tr } |A|C = \sum_n |A_n| \langle n|C|n\rangle \leq \sum_n (|A_n| \times \|C\|) = |\text{Tr } A| \times \|C\|. \blacksquare \quad (2.18)$$

Lemma 7 *Let $\{A^{(i)}\}$ be a sequence of positive trace-class operators with $A^{(i)} \rightarrow \bar{A}$ and let C be any bounded operator. If $\text{Tr } A^{(i)}C = c$ for all i then $\text{Tr } \bar{A}C = c$.*

Compare with lemma 3. In the case of a bounded operator, taking the limit preserves the trace exactly, whereas with an unbounded operator we get only an upper bound.

Proof: Since $A^{(i)} \rightarrow \bar{A}$ and using lemma 5, for any $\epsilon > 0$ we can find $\|A^{(i)} - \bar{A}\|_2$ sufficiently small that

$$|\text{Tr } (A^{(i)} - \bar{A})| < \frac{\epsilon}{\|C\|}. \quad (2.19)$$

Then by lemma 6, $\text{Tr } |A^{(i)} - \bar{A}|C < \epsilon$. Since $\text{Tr } A^{(i)}C = c$, it follows that $|\text{Tr } \bar{A}C - c| < \epsilon$ for every $\epsilon > 0$ and thus that $\text{Tr } \bar{A}C = c$ as desired.

Lemma 8 *The space $\mathcal{P}(E)$ is complete.*

Proof: Let $\{\rho^{(i)}\}$ be a Cauchy sequence of density operators in $\mathcal{P}(E)$. The space $\mathcal{P}(E)$ is part of the space of Hilbert-Schmidt operators on \mathcal{H} , which is a complete space under the $\|\cdot\|_2$ norm. Thus there is a Hilbert-Schmidt operator

$$\bar{\rho} = \lim_{i \rightarrow \infty} \rho^{(i)} \quad (2.20)$$

Clearly $\bar{\rho}$ is Hermitian. By lemma 2, $\bar{\rho} \geq 0$. By lemma 3, $\text{Tr } \bar{\rho}H \leq E$. Then by lemma 7 with $C = I$, $\text{Tr } \bar{\rho} = 1$. Thus $\bar{\rho} \in \mathcal{P}(E)$. So any Cauchy sequence in $\mathcal{P}(E)$ converges to a limit in $\mathcal{P}(E)$, which is to say that $\mathcal{P}(E)$ is complete. \blacksquare

Lemma 9 *The space $\mathcal{P}(E)$ is totally bounded, i.e. any sequence of $\rho^{(n)}$ in $\mathcal{P}(E)$ has a Cauchy subsequence.*

Proof: Let $\{\rho^{(n)}\}$, $n = 1 \dots \infty$ be an infinite sequence of operators in $\mathcal{P}(E)$. As before we work in a basis where H is diagonal. The space of Hermitian, positive, unit-trace $n \times n$ matrices is compact. Thus any sequence of such matrices has a Cauchy subsequence. So define a set of sequences of integers $\{n_k(i)\}$, $k \geq 0$ as follows: Let

$n_0(i) = i$ and for each k define $\{n_k(i)\}$ to be a subsequence of $\{n_{k-1}(i)\}$ such that $\rho^{(n_k(i))} \downarrow_k$ is a Cauchy sequence. Then let $\hat{\rho}^{(i)} = \rho^{(n_i(i))}$. We claim that $\hat{\rho}^{(i)}$ is a Cauchy sequence.

Given any $\epsilon > 0$, by lemma 4 we can find an N such that

$$\sum_{n=N}^{\infty} \rho_{nn} < \frac{\epsilon}{16} \quad (2.21)$$

for every $\rho \in \mathcal{P}(E)$. Since ρ is positive, $|\rho_{ab}|^2 < \rho_{nn}\rho_{bb}$. Thus

$$\sum_{a=1}^{\infty} \sum_{b=N}^{\infty} |\rho_{ab}|^2 \leq \sum_{a=1}^{\infty} \rho_{nn} \sum_{b=N}^{\infty} \rho_{bb} \leq \text{Tr } \rho \cdot \frac{\epsilon}{16} = \frac{\epsilon}{16}. \quad (2.22)$$

Now since $\{\rho^{(n_N(i))} \downarrow_N\}$ is a Cauchy sequence we can choose a number $M \geq N$ such that

$$\|\rho^{(n_N(i))} \downarrow_N - \rho^{(n_N(j))} \downarrow_N\|_2^2 < \epsilon/2 \quad (2.23)$$

for all $i, j \geq M$. Then

$$\begin{aligned} & \|\rho^{(n_N(i))} - \rho^{(n_N(j))}\|_2^2 - \|\rho^{(n_N(i))} \downarrow_N - \rho^{(n_N(j))} \downarrow_N\|_2^2 \\ &= \sum_{a \text{ or } b > N} \left| \rho_{ab}^{(n_N(i))} - \rho_{ab}^{(n_N(j))} \right|^2 \\ &\leq 2 \sum_{a=1}^{\infty} \sum_{b=N+1}^{\infty} \left| \rho_{ab}^{(n_N(i))} - \rho_{ab}^{(n_N(j))} \right|^2 \\ &\leq 4 \sum_{a=1}^{\infty} \sum_{b=N+1}^{\infty} \left(\left| \rho_{ab}^{(n_N(i))} \right|^2 + \left| \rho_{ab}^{(n_N(j))} \right|^2 \right) < \frac{\epsilon}{2}. \end{aligned} \quad (2.24)$$

Thus

$$\|\rho^{(n_N(i))} - \rho^{(n_N(j))}\|_2^2 \leq \epsilon \quad (2.25)$$

for all $i, j \geq M$. For any given $k \geq N$, $n_k(k)$ is $n_N(i)$ for some $i \geq k$, since the $n_k(i)$ are a subsequence of the $n_N(i)$. Thus for any $k, l \geq N$, and consequently for any $k, l \geq M$, we find that

$$\|\hat{\rho}^{(k)} - \hat{\rho}^{(l)}\|_2^2 = \|\rho^{(n_k(k))} - \rho^{(n_l(l))}\|_2^2 = \|\rho^{(n_N(i))} - \rho^{(n_N(j))}\|_2^2 \quad (2.26)$$

for some $i, j \geq M$, and thus that

$$\|\hat{\rho}^{(k)} - \hat{\rho}^{(l)}\|_2^2 < \epsilon \quad (2.27)$$

which is to say that $\hat{\rho}^{(i)}$ is a Cauchy sequence. \blacksquare

Proof of theorem 1: By lemma 9, $\mathcal{P}(E)$ is totally bounded. By lemma 8, $\mathcal{P}(E)$ is complete, which is to say that $\mathcal{P}(E)$ is compact. \blacksquare

2.1.2 Continuity of the entropy

We now prove that S is continuous if we restrict ourselves to ρ with $\text{Tr } \rho H \leq E$.

Theorem 2 $S(\rho) = -\text{Tr } \rho \ln \rho$ is continuous on $\mathcal{P}(E)$ in the $\|\cdot\|_2$ norm.

Proof: Let ρ be any density operator in $\mathcal{P}(E)$. Given any $\epsilon > 0$ we need to find a $\delta > 0$ such that $|S(\rho) - S(\rho')| < \epsilon$ for every $\rho' \in \mathcal{P}(E)$ with $\|\rho - \rho'\|_2 < \delta$. We will do this by writing ρ as the limit of $N \times N$ matrices $\rho_{\downarrow N}$ and ρ' as the limit of $\rho'_{\downarrow N}$.

We work again in a basis where H is diagonal. Since $\rho_{\downarrow N}$ is a matrix of finite dimension, $S(\rho_{\downarrow N})$ is continuous. Thus given any N we can find a δ such that

$$|S(\rho_{\downarrow N}) - S(\rho'_{\downarrow N})| < \frac{\epsilon}{3} \quad (2.28)$$

whenever $\|\rho_{\downarrow N} - \rho'_{\downarrow N}\|_2 < \delta$. Thus it is sufficient to find an N such that $|S(\rho_{\downarrow N}) - S(\rho)| < \epsilon/3$ for all $\rho \in \mathcal{P}(E)$.

Let $p_k(\rho)$ denote the k th largest eigenvalue of ρ . Lieb, Ruskai and Simon [34] show that $p_k(\rho_{\downarrow N}) \leq p_k(\rho)$, and go on to show from this that

$$\lim_{N \rightarrow \infty} S(\rho_{\downarrow N}) = S(\rho). \quad (2.29)$$

We want to extend this result to show that $S(\rho_{\downarrow N}) \rightarrow S(\rho)$ uniformly for all ρ such that $\text{Tr } \rho H \leq E$.

Define the function

$$s(p) = \begin{cases} -p \ln p & p > 0 \\ 0 & p = 0. \end{cases} \quad (2.30)$$

Note that s is continuous. It is increasing for $p < 1/e$ and decreasing for $p > 1/e$. As we go from $S(\rho_{\downarrow N})$ to $S(\rho)$ the p_k will increase. It is possible to have a few large p_k such that increasing p_k will decrease $s(p_k)$, but for the majority of p_k an increase in p_k means an increase in $s(p_k)$.

First we study how much S can decrease as $N \rightarrow \infty$. Let ϵ be any small positive number. By lemma 4 we can find N_- large enough so that

$$\sum_{a=N_-}^{\infty} \rho_{nn} < \frac{\epsilon}{3} \quad (2.31)$$

for every $\rho \in \mathcal{P}(E)$. Thus

$$\text{Tr } \rho_{\downarrow N} = 1 - \sum_{n=N+1}^{\infty} \rho_{nn} > 1 - \frac{\epsilon}{3} \quad (2.32)$$

for any $N > N_-$. Now $\sum p_k(\rho) = \text{Tr } \rho = 1$, so

$$\sum_k (p_k(\rho) - p_k(\rho_{\downarrow N})) < \frac{\epsilon}{3}. \quad (2.33)$$

Since $ds/dp \geq -1$ for all $p \leq 1$, we can conclude that

$$S(\rho_{\downarrow N}) - S(\rho) < \frac{\epsilon}{3} \quad (2.34)$$

for all $N > N_-$.

Now we study how much S can increase as $N \rightarrow \infty$. We write

$$\rho = \left(\begin{array}{c|c} \rho_{\downarrow N} & A \\ \hline A^T & \rho_{\uparrow N} \end{array} \right). \quad (2.35)$$

For fixed $\rho_{\downarrow N}$ and $\rho_{\uparrow N}$, $S(\rho)$ will be largest when $A = 0$. To see this, consider

$$\rho_- = \left(\begin{array}{c|c} \rho_{\downarrow N} & -A \\ \hline -A^T & \rho_{\uparrow N} \end{array} \right). \quad (2.36)$$

The eigenvalues of ρ_- are the same as those of ρ , so $S(\rho) = S(\rho_-)$. Now let

$$\rho_0 = \left(\begin{array}{c|c} \rho_{\downarrow N} & 0 \\ \hline 0 & \rho_{\uparrow N} \end{array} \right) = \frac{\rho + \rho_-}{2}. \quad (2.37)$$

Since the entropy is convex (see [35] and section 2.2.3), $S(\rho_0) > (S(\rho) + S(\rho_-))/2 = S(\rho)$. Thus $S(\rho) < S(\rho_0) = S(\rho_{\downarrow N}) + S(\rho_{\uparrow N})$.

Now $\rho_{\uparrow N}$ obeys the constraints

$$\text{Tr } \rho_{\uparrow N} = 1 - \text{Tr } \rho_{\downarrow N} \equiv 1 - p_< \quad (2.38a)$$

$$\text{Tr } \rho_{\uparrow N} H \leq E - \text{Tr } \rho_{\downarrow N} H \equiv E_>. \quad (2.38b)$$

Let $S_{\text{th}}(E; e_1, e_2, e_3, \dots)$ denote the thermal entropy of a system whose energy levels are e_1, e_2, e_3, \dots . Suppose we had a system with energy levels $0, E_{N+1}, E_{N+2}, \dots$. Then a possible normalized density matrix would be

$$\left(\begin{array}{c|c} p_< & 0 \\ \hline 0 & \rho_{\uparrow N} \end{array} \right). \quad (2.39)$$

It would have energy $E_> < E$ and entropy $-p_< \ln p_< + S(\rho_{\uparrow N})$. This must be less than the maximum entropy for this system with energy $\leq E$, so we conclude that

$$S(\rho) - S(\rho_{\downarrow N}) < S(\rho_{\uparrow N}) < S_{\text{th}}(E; 0, E_{N+1}, E_{N+2}, \dots). \quad (2.40)$$

Now as $N \rightarrow \infty$, only higher and higher energy states are permitted in the expression above, so the entropy will decrease to zero. That is,

$$\lim_{N \rightarrow \infty} S_{\text{th}}(E; 0, E_{N+1}, E_{N+2}, \dots) = 0. \quad (2.41)$$

So, given $\epsilon > 0$ we can find N_+ such that if $N > N_+$ then

$$S(\rho) - S(\rho \downarrow_N) < \frac{\epsilon}{3} \quad (2.42)$$

for any $\rho \in \mathcal{P}(E)$.

Now we set $N = \max(N_+, N_-)$. From Eqs. (2.34) and (2.42) we find that

$$|S(\rho) - S(\rho \downarrow_N)| < \frac{\epsilon}{3}, \quad (2.43)$$

for every $\rho \in \mathcal{P}(E)$. Then we choose δ as in Eq. (2.28). If $\|\rho - \rho'\|_2 < \delta$ then

$$|S(\rho) - S(\rho')| < |S(\rho) - S(\rho \downarrow_N)| + |S(\rho \downarrow_N) - S(\rho' \downarrow_N)| + |S(\rho' \downarrow_N) - S(\rho')| < \epsilon. \blacksquare \quad (2.44)$$

Theorem 3 *Let \mathcal{H} and H be defined as in theorem 1, let $\{C_\alpha\}$ be a set of positive operators with discrete spectra, and let $\mathcal{P}_{\leq}(E; V_1, V_2, \dots)$ be the set of density operators ρ such that $\text{Tr} \rho H \leq E$ and $\text{Tr} \rho C_\alpha \leq V_\alpha$ for all α . Then $S(\rho)$ achieves a maximum on $\mathcal{P}_{\leq}(E; V_1, V_2, \dots)$.*

Proof: From theorem 1 we know that $\mathcal{P}(E)$ is compact. Thus any sequence of $\rho^{(n)} \in \mathcal{P}_{\leq}(E; V_1, V_2, \dots)$ has a subsequence that converges to some $\bar{\rho} \in \mathcal{P}(E)$. By repeated application of lemma 3 we see that $\text{Tr} \bar{\rho} C_\alpha \leq V_\alpha$ so $\bar{\rho} \in \mathcal{P}_{\leq}(E; V_1, V_2, \dots)$. Thus $\mathcal{P}_{\leq}(E; V_1, V_2, \dots)$ is sequentially compact, and so it is compact. By theorem 2, S is continuous on $\mathcal{P}(E)$, so S achieves a maximum on $\mathcal{P}_{\leq}(E; V_1, V_2, \dots)$. \blacksquare

It is possible to rearrange the constraints that we will need into positive operators. However, our constraints are of the type $\text{Tr} \rho C_\alpha = V_\alpha$ rather than $\text{Tr} \rho C_\alpha \leq V_\alpha$. What we really need is

Conjecture 1 *Define \mathcal{H} , H and $\{C_\alpha\}$ as in theorem 3 and let $\mathcal{P}_=(E; V_1, V_2, \dots)$ be the set of density operators ρ such that $\text{Tr} \rho H = E$ and $\text{Tr} \rho C_\alpha = V_\alpha$ for all α . Then $S(\rho)$ achieves a maximum on $\mathcal{P}_=(E; V_1, V_2, \dots)$.*

Unfortunately, we do not know how to complete the proof of this conjecture. However, in the next section we show that if there is such a ρ it is unique. Furthermore since $\mathcal{P}_=(E; V_1, V_2, \dots) \subset \mathcal{P}_{\leq}(E; V_1, V_2, \dots)$ the maximum value of S in theorem 3 is at worst an upper bound on $S(\rho)$ with $\rho \in \mathcal{P}_=(E; V_1, V_2, \dots)$.

2.2 Maximization of the entropy

To maximize the entropy we would like to look at the variation of S as ρ is varied and require that $\delta S = 0$ so that S can be a maximum. However, when ρ is varied we may find that δS is not well-defined. There are two possible causes for this. One is that ρ has some zero eigenvalues. The second is that ρ has arbitrarily small eigenvalues which become negative under any variation. We treat these problems below.

First, since we are concerned with zero eigenvalues we should specify what we mean by S . When we write $S(\rho) = -\text{Tr} \rho \ln \rho$ we mean that $S(\rho) = s(\rho)$, where s is

defined in Eq. (2.30). That is, if $\rho = \sum P_\alpha |\alpha\rangle\langle\alpha|$ then $S = \sum s(P_\alpha)$ or alternatively if we write $s(p)$ as a power series in p then $S(\rho)$ is given by the same power series in ρ . Under this definition $S(\rho)$ is well-defined when ρ has zero eigenvalues, even though $\ln \rho$ is not defined in such cases.

2.2.1 Variation of S

We want to vary ρ via $\rho' = \rho + t\delta\rho$ and look at the resulting change in $S(\rho')$. We will call a variation $\delta\rho$ admissible if:

- $\delta\rho$ is Hermitian.
- $\text{Tr } \delta\rho = 0$, so that $\text{Tr } \rho' = 1$.
- For each α , $\text{Tr } \delta\rho C_\alpha = 0$, so that $\text{Tr } \rho' C_\alpha$ is unchanged.
- For sufficiently small $t > 0$, $\rho' \geq 0$.

Under these conditions ρ' is a well-defined density operator for at least some small range of $t > 0$.

We will often want to let $\delta\rho$ interpolate between ρ and some other density operator $\bar{\rho}$. To show that this is always possible, we prove

Theorem 4 *The space of density operators ρ that obey the constraints is convex, i.e. if ρ and $\bar{\rho}$ are density operators that obey the constraints then $\delta\rho = \bar{\rho} - \rho$ is an admissible variation and $\rho_0 = \rho + t\delta\rho$ is a density operator for all $t \in [0, 1]$.*

Proof:

- Since ρ and $\bar{\rho}$ are Hermitian, so is $\delta\rho$.
- $\text{Tr } \delta\rho = \text{Tr } \bar{\rho} - \text{Tr } \rho = 0$.
- $\text{Tr } \delta\rho C_\alpha = \text{Tr } \bar{\rho} C_\alpha - \text{Tr } \rho C_\alpha = 0$.
- Let \mathbf{x} be any state vector. Then for all $t \in [0, 1]$, $\mathbf{x} \cdot \rho' \mathbf{x} = \mathbf{x} \cdot (t\bar{\rho} + (1-t)\rho) \mathbf{x} = t(\mathbf{x} \cdot \bar{\rho} \mathbf{x}) + (1-t)(\mathbf{x} \cdot \rho \mathbf{x}) \geq 0$, i.e. $\rho' \geq 0$. ■

Now

$$S(\rho) = \sum_\alpha s(p_\alpha) \quad (2.45)$$

where p_α are the eigenvalues of ρ . When we vary ρ , the change in the eigenvalues is given by first-order perturbation theory,

$$\frac{dp_\alpha}{dt} = \langle \alpha | \delta\rho | \alpha \rangle = \delta\rho_{\alpha\alpha}. \quad (2.46)$$

If $p_\alpha > 0$ then we have

$$\frac{ds(p_\alpha)}{dp_\alpha} = -(1 + \ln p_\alpha). \quad (2.47)$$

Thus if there are no zero eigenvalues we can write

$$\frac{dS}{dt} = - \sum_{\alpha} (1 + \ln p_{\alpha}) \delta \rho_{\alpha} = -\text{Tr} \delta \rho - \text{Tr} \delta \rho \ln \rho' = -\text{Tr} \delta \rho \ln \rho', \quad (2.48)$$

since we have required $\text{Tr} \delta \rho = 0$.

2.2.2 Prohibited sectors

If there are zero eigenvalues, then $\ln \rho$ and thus Eq. (2.48) are not well-defined. We handle this case as follows:

Theorem 5 *If ρ maximizes S subject to the constraints $\text{Tr} \rho C_{\alpha} = V_{\alpha}$ and if $\rho |\alpha\rangle = 0$, then every ρ that satisfies the constraints must annihilate $|\alpha\rangle$.*

Proof: Suppose to the contrary that $\rho |\alpha\rangle = 0$ but there is some $\bar{\rho}$ such that $\text{Tr} \bar{\rho} C_{\alpha} = V_{\alpha}$ but $\bar{\rho} |\alpha\rangle \neq 0$. We let $\delta \rho = \bar{\rho} - \rho$. By theorem 4, $\delta \rho$ is admissible. Now we look at just those p_{α} that are in fact changed by $\delta \rho$. Let t be some small but positive number. Then all the p_{α} that are changed by $\delta \rho$ are positive and we can write

$$\frac{dS}{dt} = - \sum_{\alpha \text{ with } \delta \rho_{\alpha} \neq 0} \delta \rho_{\alpha} \ln \rho_{\alpha}. \quad (2.49)$$

As $t \rightarrow 0$ the $-\ln p_{\alpha}$ terms grow without bound for those α where $p_{\alpha}(t) \rightarrow 0$. Thus eventually these terms dominate everything else in Eq. (2.49) so that

$$\lim_{t \rightarrow 0} \frac{dS}{dt} = +\infty. \quad (2.50)$$

Thus for sufficiently small $t > 0$ there is a $\bar{\rho}$ with $S(\bar{\rho}) > S(\rho)$ in contradiction to assumption. Thus if ρ maximizes S then we must have $\bar{\rho} |\alpha\rangle = 0$ for every $|\alpha\rangle$ where $\rho |\alpha\rangle = 0$. ■

Thus ρ can have a nontrivial nullspace $\mathcal{N} \subset \mathcal{H}$ only if every ρ that satisfies the constraints annihilates the space \mathcal{N} . In this case, we will write $\mathcal{H} = \mathcal{N} \oplus \mathcal{H}'$ and work in the space \mathcal{H}' . We will replace all our operators with ones that act only on \mathcal{H}' . If, restricted to \mathcal{H}' , the constraints are linearly dependent, we can now discard some of them to have again a linearly independent set. This process eliminates the troublesome sector from the problem.

2.2.3 Derivatives of S

If $\delta \rho$ is an admissible variation, and as long as there are no zero eigenvalues, we can differentiate S with respect to t as in Eq. (2.48). We demand that

$$\frac{dS}{dt} = -\text{Tr} \delta \rho \ln \rho' = 0 \quad (2.51)$$

for S to be a maximum.

For the second derivative we care only about the sign. Lieb [35] showed that S is always (downward) concave. Here we obtain the same result by a different technique and show also that the concavity is strict, i.e. that

$$\frac{d^2S}{dt^2} < 0 \quad (2.52)$$

for any ρ and any nonzero $\delta\rho$.

From Eq. (2.51)

$$\frac{d^2S}{dt^2} = -\text{Tr } \delta\rho \frac{d}{dt} \ln \rho'. \quad (2.53)$$

To expand this we use the formula

$$\frac{d}{dt} \ln A = \int_0^1 ds (I - s(A - I))^{-1} \frac{dA}{dt} (I - s(A - I))^{-1} \quad (2.54)$$

which can easily be derived as follows: Let $B = A - I$. We expand

$$\ln A = \ln(I + B) = B + \frac{B^2}{2} + \frac{B^3}{3} + \dots \quad (2.55)$$

and differentiate to get

$$\begin{aligned} \frac{d}{dt} \ln A &= \frac{dB}{dt} + \frac{1}{2} \left(\frac{dB}{dt} B + B \frac{dB}{dt} \right) \\ &\quad + \frac{1}{3} \left(\frac{dB}{dt} B^2 + B \frac{dB}{dt} B + B^2 \frac{dB}{dt} \right) + \dots \end{aligned} \quad (2.56)$$

We observe that this is

$$\begin{aligned} &\int_0^1 ds \frac{dB}{dt} + s \left(\frac{dB}{dt} B + B \frac{dB}{dt} \right) + s^2 \left(\frac{dB}{dt} B^2 + B \frac{dB}{dt} B + B^2 \frac{dB}{dt} \right) \\ &= \int_0^1 ds (1 + sB + s^2 B^2 + \dots) \frac{dB}{dt} (1 + sB + s^2 B^2 + \dots) \\ &= \int_0^1 ds (I - sB)^{-1} \frac{dB}{dt} (I - sB)^{-1} \end{aligned} \quad (2.57)$$

as desired.

Using Eq. (2.54) we find

$$\begin{aligned} \frac{d^2S}{dt^2} &= - \int_0^1 ds \text{Tr } \delta\rho (I - s(\rho - I))^{-1} \delta\rho (I - s(\rho - I))^{-1} \\ &= - \int_0^1 \text{Tr } X(s)^2 \end{aligned} \quad (2.58)$$

where

$$X(s) \equiv (\delta\rho)^{1/2}(I - s(\rho - I))^{-1}(\delta\rho)^{1/2}. \quad (2.59)$$

Since $X(s)$ is Hermitian, $\text{Tr } X(s)^2 \geq 0$ with equality obtained only for $X(s) = 0$. Thus

$$\frac{dS^2}{dt^2} \leq 0 \quad (2.60)$$

with equality only if $X(0) = 0$ for all s . But $X(0) = \delta\rho$, and thus

$$\frac{dS^2}{dt^2} < 0 \quad (2.61)$$

for any nonzero $\delta\rho$.

Now suppose that ρ maximizes S . Then for any admissible $\delta\rho$, we must have

$$\frac{dS}{dt} \leq 0 \quad (2.62)$$

or else for sufficiently small t we would have $S(\rho') > S(\rho)$. Furthermore we can see that condition (2.62) is sufficient to show that ρ maximizes S , as follows: Let $\bar{\rho}$ be any other density operator that meets the constraints. Let $\delta\rho = \bar{\rho} - \rho$. From theorem 4, $\delta\rho$ is admissible. From Eqs. (2.62) and (2.52), it follows that $S(\bar{\rho}) < S(\rho)$. Since this holds for any $\bar{\rho}$, ρ is the global maximum of S . It follows from this that if there is a ρ in conjecture 1 it is unique.

2.3 The form of ρ

We must find the unique state ρ (if any) which satisfies our constraints and which gives $\text{Tr } \delta\rho \ln \rho = 0$ for any $\delta\rho$ which maintains the constraints. This means that we are concerned with $\delta\rho$ such that

$$\text{Tr } \delta\rho = 0 \quad (2.63a)$$

$$\text{Tr } \delta\rho C_\alpha = 0 \quad (2.63b)$$

for all α . We have included the Hamiltonian among the constraints C_α . For every $\delta\rho$ satisfying Eqs. (2.63) we must have

$$\text{Tr } \delta\rho \ln \rho = 0. \quad (2.64)$$

If we choose

$$\ln \rho = \text{const} + \sum_\alpha f_\alpha C_\alpha \quad (2.65)$$

which is to say

$$\rho \propto e^{\sum f_\alpha C_\alpha}, \quad (2.66)$$

with any coefficients f_α , then Eqs. (2.63) ensure that Eq. (2.64) is satisfied. If we can find a ρ with the form of Eq. (2.66) that satisfies the constraints, then we have found the unique solution. We have not shown that such a solution always exists, but in the numerical work described in section 4.3 we have always succeeded in finding one.

Since $\text{Tr } \rho = 1$, we can write

$$\rho = \frac{e^{\sum f_\alpha C_\alpha}}{\text{Tr } e^{\sum f_\alpha C_\alpha}}. \quad (2.67)$$

Our goal is now to determine the coefficients f_α so that the constraints are satisfied.

We can define a grand partition function,

$$Q = \text{Tr } e^{\sum f_\alpha C_\alpha}. \quad (2.68)$$

Its derivatives are

$$\frac{dQ}{df_\alpha} = \text{Tr } C_\alpha e^{\sum f_\alpha C_\alpha}, \quad (2.69)$$

so

$$\langle C_\alpha \rangle = \frac{d}{df_\alpha} \ln Q. \quad (2.70)$$

We have the usual thermodynamic formula for the entropy,

$$S = -\langle \ln \rho \rangle = \ln Q - \sum f_\alpha \langle C_\alpha \rangle. \quad (2.71)$$

Differentiating this we find

$$\frac{dS}{df_\alpha} = - \sum f_\beta \frac{d\langle C_\beta \rangle}{df_\alpha}. \quad (2.72)$$

Now we specialize to the case where one of the constraints is just the Hamiltonian. The corresponding coefficient is written $-\beta$, and we have

$$\rho = \frac{1}{Q} e^{-\beta H + \sum f_\alpha C_\alpha}. \quad (2.73)$$

If we vary the coefficients in such a way that $\langle H \rangle = E$ changes but the other $\langle C_\alpha \rangle = V_\alpha$ remain fixed we see that

$$dS = - \sum f_\alpha d\langle C_\alpha \rangle = \beta dE. \quad (2.74)$$

Thus $\beta = dS/dE$ and so the coefficient β has the usual interpretation as the inverse temperature.

Chapter 3

The Problem

Now we return to the problem at hand. We would like to find the maximum-entropy vacuum-bounded state with a given average energy E_0 . We first reduce the problem to a simpler case which we hope will capture the important behavior. Then we analyze the sectors on which ρ must be zero and introduce new coordinates in which these sectors do not appear. We work with these new coordinates to derive formulas for the expectation values of the operators that must agree with the vacuum. Finally we look at the form of the results to be expected when we solve the problem numerically in the next chapter.

3.1 Simplifications

3.1.1 One scalar field, one dimension

First we restrict ourselves to a theory consisting only of gravity and one massless scalar field. In such a system we can imagine preparing an incoming shell of scalar particles to form a black hole, which would then evaporate by emitting scalar quanta. Thus we can ask the same questions about black hole evaporation in this system as we could, say, in the standard model plus gravity.

We will also begin here by working in one dimension. We will put our entire system in a box of length L and require that all deviations from the vacuum are in the region from 0 to L_{in} . Later we will take the overall box size L to infinity while L_{in} remains fixed. The inside region will be $[0, L_{\text{in}}]$ and the outside region will be $[L_{\text{in}}, L]$. We will use the usual scalar field Hamiltonian, which in classical form is

$$H = \frac{1}{2} \int_0^L \left[\pi(x)^2 + \left(\frac{d\phi}{dx} \right)^2 \right] dx. \quad (3.1)$$

3.1.2 Gaussian form

In our problem, the constraints are the energy bound,

$$\mathrm{Tr} \rho H = E_0, \quad (3.2)$$

and the vacuum-bounded condition,

$$\mathrm{Tr} \rho O_{\text{out}}^\alpha = \langle 0 | O_{\text{out}}^\alpha | 0 \rangle, \quad (3.3)$$

where O_{out}^α is any operator which is constructed out of the fields $\phi(x)$ and $\pi(x)$ in the outside region. We will assume the solution has the form

$$\rho \propto e^{-\beta H + \sum f_\alpha O_{\text{out}}^\alpha}. \quad (3.4)$$

We now show that f_α is nonzero only for those operators O_{out}^α which are quadratic in the fields.

Suppose that we wanted to solve a different problem in which we cared only about the constraints involving the quadratic operators. We would have the energy bound and the constraints

$$\mathrm{Tr} \rho Q_{\text{out}}^a = \langle 0 | Q_{\text{out}}^a | 0 \rangle, \quad (3.5)$$

where Q_{out}^a runs only over quadratic operators $\phi(x)\phi(y)$ and $\pi(x)\pi(y)$. (The operators $\phi(x)\pi(y)$ vanish automatically by symmetry under $\phi \rightarrow -\phi$.) We expect the solution to this problem to have the form

$$\rho' \propto e^{-\beta H + \sum f_a Q_{\text{out}}^a}. \quad (3.6)$$

Now ρ' is a Gaussian operator; i.e., $\langle \phi(\cdot) | \rho' | \phi'(\cdot) \rangle$ is a Gaussian functional of the values of ϕ and ϕ' . Let $\rho'_{\text{out}} = \mathrm{Tr}_{\text{in}} \rho'$. The trace is just a set of Gaussian integrals, which means that the resulting ρ'_{out} is also a Gaussian. Because H is quadratic, the vacuum $\rho^{\text{vac}} = |0\rangle\langle 0|$ is Gaussian, and so is its trace $\rho'_{\text{out}}^{\text{vac}} = \mathrm{Tr}_{\text{in}} \rho^{\text{vac}}$. Now by construction we have $\mathrm{Tr} \rho'_{\text{out}} \phi(x)\phi(y) = \mathrm{Tr} \rho_{\text{out}}^{\text{vac}} \phi(x)\phi(y)$ and $\mathrm{Tr} \rho'_{\text{out}} \pi(x)\pi(y) = \mathrm{Tr} \rho_{\text{out}}^{\text{vac}} \pi(x)\pi(y)$. These conditions are sufficient to fix the coefficients in the Gaussian ρ'_{out} , and thus to show that in fact ρ'_{out} and $\rho_{\text{out}}^{\text{vac}}$ are the same Gaussian; i.e. that $\mathrm{Tr}_{\text{in}} \rho' = \mathrm{Tr}_{\text{in}} \rho^{\text{vac}}$.

Thus ρ' satisfies all the constraints of the original problem. Since only one ρ can have these properties it follows that $\rho = \rho'$ and thus that Gaussian solution ρ' is the correct solution to the original problem.

3.1.3 The discrete case

We now approximate the continuum by a one-dimensional lattice of coupled oscillators, with a classical Hamiltonian

$$H = \frac{1}{2} (\mathbf{P}_x \cdot \mathbf{P}_x + \mathbf{x} \cdot K \mathbf{x}). \quad (3.7)$$

The simple kinetic term in Eq. (3.7) corresponds to choosing oscillators of unit mass, regardless of how densely they are packed. In terms of scalar-field variables this means that $x_\mu = \sqrt{L_1}\phi_\mu$ and $P_\mu = \pi_\mu/\sqrt{L_1}$ where $L_1 = L/(N+1)$ is the lattice spacing, ϕ_μ is the average of $\phi(x)$ over an interval of length L_1 , and π_μ is the total momentum $\pi(x)$ in the interval.

The matrix K gives the couplings between the oscillators and represents the $d\phi/dx$ term in the scalar field Hamiltonian. To approximate the continuum with the zero-field boundary condition we will imagine that we have N oscillators located at the points $1/(N+1) \dots N/(N+1)$ and that the end oscillators are coupled to fixed-zero oscillators at 0 and 1. Then

$$K = \begin{pmatrix} 2g & -g & 0 & 0 & \cdot \\ -g & 2g & -g & 0 & \cdot \\ 0 & -g & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \quad (3.8)$$

where $g = 1/L_1^2$.

We will take $N_{\text{in}} \approx L_{\text{in}}/L_1$ of the oscillators to represent the inside region, and $N_{\text{out}} = N - N_{\text{in}}$ to represent the outside region.

We want to maximize S subject to the constraints

$$\text{Tr } \rho H = E_0 \quad (3.9a)$$

$$\text{Tr } \rho x_i x_j = \langle 0 | x_i x_j | 0 \rangle \quad (3.9b)$$

$$\text{Tr } \rho P_i P_j = \langle 0 | P_i P_j | 0 \rangle, \quad (3.9c)$$

where i and j run over the oscillators which represent the outside region. We will define matrices \mathbb{X} and \mathbb{P} whose elements are the quadratic operators via

$$\mathbb{X}_{\mu\nu} = x_\mu x_\nu \quad (3.10a)$$

$$\mathbb{P}_{\mu\nu} = P_\mu P_\nu \quad (3.10b)$$

so that Eqs. (3.9b) and (3.9c) become

$$\text{Tr } \rho \mathbb{X}_{\text{out,out}} = \langle 0 | \mathbb{X}_{\text{out,out}} | 0 \rangle \quad (3.11a)$$

$$\text{Tr } \rho \mathbb{P}_{\text{out,out}} = \langle 0 | \mathbb{P}_{\text{out,out}} | 0 \rangle. \quad (3.11b)$$

3.2 Prohibited sectors

As discussed in section 2.2.2, the first thing we need to do is to look for sectors of our Hilbert space that any ρ must annihilate in order to meet the constraints, and restrict our attention to the subspace orthogonal to these. We will start by examining the ground state of our system and looking for sectors which are forced to remain in the ground state.

3.2.1 A different description of the vacuum

To work with the Hamiltonian of Eq. (3.7) we will make a change of coordinate to put it in diagonal form. Let Z be a matrix whose columns are the eigenvectors of K , $K = Z\Omega_0^2 Z^{-1}$, with the normalization

$$Z\Omega_0 Z^T = I \quad \text{and} \quad Z^{-1^T} \Omega_0 Z^{-1} = K. \quad (3.12)$$

Define new coordinates \mathbf{z} via $\mathbf{x} = Z\mathbf{z}$ and $\mathbf{P}_x = Z^{-1^T} \mathbf{P}_z$. In these coordinates,

$$H = \frac{1}{2} \sum_{\alpha} \omega_{\alpha}^{(0)} (P_{z_{\alpha}}^2 + z_{\alpha}^2). \quad (3.13)$$

The vacuum is the ground state of this Hamiltonian. We can define raising and lowering operators

$$a_{\alpha} = \frac{1}{\sqrt{2}} (z_{\alpha} + iP_{z_{\alpha}}) \quad (3.14a)$$

$$a_{\alpha}^{\dagger} = \frac{1}{\sqrt{2}} (z_{\alpha} - iP_{z_{\alpha}}) \quad (3.14b)$$

$$H = \sum_{\alpha} \omega_{\alpha}^{(0)} \left(a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{2} \right). \quad (3.14c)$$

The vacuum is the state $|0\rangle$ annihilated by all the a_{α} . It is straightforward to write the expectation values in the vacuum state,

$$\langle \mathbb{Z} \rangle_{\alpha\beta} \equiv \langle 0 | z_{\alpha} z_{\beta} | 0 \rangle = \frac{1}{2} \delta_{\alpha\beta} \quad (3.15a)$$

$$\langle \mathbb{P}_z \rangle_{\alpha\beta} \equiv \langle 0 | P_{z_{\alpha}} P_{z_{\beta}} | 0 \rangle = \frac{1}{2} \delta_{\alpha\beta} \quad (3.15b)$$

so

$$\langle 0 | \mathbb{X} | 0 \rangle = Z \langle 0 | \mathbb{Z} | 0 \rangle Z^T = \frac{1}{2} Z Z^T \quad (3.16a)$$

$$\langle 0 | \mathbb{P} | 0 \rangle = Z^{-1^T} \langle 0 | \mathbb{P}_z | 0 \rangle Z^{-1} = \frac{1}{2} Z^{-1^T} Z^{-1} = \frac{1}{4} (\langle 0 | \mathbb{X} | 0 \rangle)^{-1}. \quad (3.16b)$$

There can be many different Hamiltonians that have the same ground state. If we consider

$$H' = \frac{1}{2} (\mathbf{P}_x \cdot T' \mathbf{P}_x + \mathbf{x} \cdot K' \mathbf{x}) \quad (3.17)$$

with T' and K' some coupling matrices, we can follow the above derivation to get a normal mode matrix Y and some frequencies Ω with

$$Y \Omega Y^T = T' \quad (3.18a)$$

$$Y^{-1^T} \Omega Y^{-1} = K' \quad (3.18b)$$

$$\mathbf{x} = Y\mathbf{y} \quad (3.18c)$$

$$\mathbf{P}_x = Y^{-1} \mathbf{P}_y \quad (3.18d)$$

$$H' = \frac{1}{2} \sum_{\beta} \omega_{\beta} \left(P_{y_{\beta}}^2 + y_{\beta}^2 \right). \quad (3.18e)$$

We can define raising and lowering operators for these modes,

$$b_{\beta} = \frac{1}{\sqrt{2}} (y_{\beta} + i P_{y_{\beta}}) \quad (3.19a)$$

$$b_{\beta}^{\dagger} = \frac{1}{\sqrt{2}} (y_{\beta} - i P_{y_{\beta}}) \quad (3.19b)$$

$$H' = \sum_{\beta} \omega_{\beta} \left(b_{\beta}^{\dagger} b_{\beta} + \frac{1}{2} \right). \quad (3.19c)$$

Now $\mathbf{y} = Y^{-1}\mathbf{x} = Y^{-1}Z\mathbf{z} = W^{-1}\mathbf{z}$ where

$$W \equiv Z^{-1}Y. \quad (3.20)$$

Similarly, $\mathbf{P}_y = Y^T \mathbf{P}_x = Y^T Z^{-1} \mathbf{P}_z = W^T \mathbf{P}_z$. Consequently,

$$\begin{aligned} b_{\beta} &= \frac{1}{\sqrt{2}} (W_{\beta\alpha}^{-1} z_{\alpha} + i W_{\beta\alpha}^T P_{z_{\alpha}}) \\ &= \frac{1}{2} (W_{\beta\alpha}^{-1} (a_{\alpha} + a_{\alpha}^{\dagger}) + W_{\beta\alpha}^T (a_{\alpha} - a_{\alpha}^{\dagger})) \\ &= \frac{1}{2} ((W^{-1} + W^T)_{\beta\alpha} a_{\alpha} + (W^{-1} - W^T)_{\beta\alpha} a_{\alpha}^{\dagger}). \end{aligned} \quad (3.21)$$

For H and H' to have the same vacuum we require that the b_{β} depend only on the a_{α} and not on the a_{α}^{\dagger} , which is to say that $W^{-1} = W^T$, i.e. that W is a unitary matrix. With W unitary, $YY^T = ZZ^T$ so the vacuum expectation values of Eq. (3.16) have the same values expressed in terms of Y as they had in terms of Z .

3.2.2 Modes that remain in the ground state

Now consider a unitary matrix W and let $Y = ZW$ as in the last section. Suppose we can find W such that Y has the following property:

The N modes can be divided into $N_{\text{gs}} > 0$ “ground state” modes and $N_{\text{free}} \equiv N - N_{\text{gs}}$ “free” modes such that for all $a \leq N_{\text{in}}$ and for all $\beta > N_{\text{free}}$, $Y_{a\beta} = 0$ and $Y_{\beta a}^{-1} = 0$.

That is to say Y and Y^{-1} will have the form

$$Y = \left(\begin{array}{c|c} N_{\text{free}} & N_{\text{gs}} \\ \hline Y_{\text{in},\text{free}} & 0 \\ \hline Y_{\text{out},\text{free}} & Y_{\text{out},\text{gs}} \end{array} \right) \}_{N_{\text{in}}} \}_{N_{\text{out}}} \quad (3.22)$$

and

$$Y^{-1} = \left(\begin{array}{c|c} N_{\text{in}} & N_{\text{out}} \\ \hline Y_{\text{free,in}}^{-1} & Y_{\text{free,out}}^{-1} \\ \hline 0 & Y_{\text{gs,out}}^{-1} \end{array} \right) \}_{N_{\text{free}}} \}_{N_{\text{gs}}} . \quad (3.23)$$

If this is the case, then for $\beta > N_{\text{free}}$, $b_\beta = (Y_{\beta\gamma}^{-1} x_\gamma + i Y_{\gamma\beta} P_{x_\gamma}) / \sqrt{2}$ depends only on outside operators x_i and P_{x_i} . In any vacuum-bounded state, regardless of entropy considerations, $\langle x_i x_j \rangle$ and $\langle P_i P_j \rangle$ have their vacuum values. Consequently, for all $\beta > N_{\text{free}}$, if ρ describes a vacuum-bounded state then $\text{Tr} \rho b_\beta^\dagger b_\beta = \langle 0 | b_\beta^\dagger b_\beta | 0 \rangle = 0$. The vacuum-bounded constraint forces modes $\beta > N_{\text{free}}$ to be in their ground states. These modes will not contribute to the calculation of the maximum-entropy vacuum-bounded state.

How many such modes can exist? Let W_β denote a column of W with $\beta > N_{\text{free}}$ and let Z^a denote a row of Z with $a \leq N_{\text{in}}$. Similarly let $(Z^{-1})_a$ denote a column of Z^{-1} . Since $Y = ZW$, $Y_{a\beta} = 0$ whenever W_β is orthogonal to Z^a . Similarly $Y^{-1} = W^T Z^{-1}$ so $Y_{\beta a}^{-1} = 0$ whenever W_β is orthogonal to $(Z^{-1})_a$. Since W is unitary, the W_β must also be orthogonal to each other. Thus there are N_{gs} columns of W which have to be orthogonal to N_{in} rows of Z , to N_{in} columns of Z^{-1} , and to each other. Since there are N components in a column of W it can be orthogonal in general to at most $N - 1$ other vectors. Thus N_{gs} is limited by $N - 1 = 2N_{\text{in}} + N_{\text{gs}} - 1$, or $N_{\text{gs}} = N - 2N_{\text{in}} = N_{\text{out}} - N_{\text{in}}$. Thus whenever $N_{\text{out}} > N_{\text{in}}$ there will be $N_{\text{gs}} = N_{\text{out}} - N_{\text{in}}$ modes that are forced to remain in the ground state.

These conditions determine the columns W_β with $\beta > 2N_{\text{in}}$ up to a unitary transformation on these columns alone, and likewise the remaining columns are determined up to a unitary matrix which combines them.

3.2.3 Density matrix and entropy

We can write $\mathcal{H} = \tilde{\mathcal{H}} \otimes \mathcal{G}$ where $\tilde{\mathcal{H}}$ is the Hilbert space of states of the “free” modes and \mathcal{G} is the Hilbert space of states of the “ground state” modes. Let $|0\rangle_{\text{gs}} \in \mathcal{G}$ denote the ground state of this system. For any operator A we can define an operator \tilde{A} that acts on $\tilde{\mathcal{H}}$ via $\langle \tilde{\alpha} | \tilde{A} | \tilde{\beta} \rangle = \langle \tilde{\alpha} \otimes 0_{\text{gs}} | A | \tilde{\beta} \otimes 0_{\text{gs}} \rangle$ for all $\tilde{\alpha}, \tilde{\beta} \in \tilde{\mathcal{H}}$.

Let ρ describe a vacuum-bounded state and let $\rho_{\text{gs}} = \text{Tr}_{\text{free}} \rho$. Then $\text{Tr} \rho_{\text{gs}} b_\beta^\dagger b_\beta = 0$. This defines the vacuum state, so $\rho_{\text{gs}} = |0\rangle_{\text{gs}} \langle 0|_{\text{gs}}$ and thus

$$\rho = \tilde{\rho} \otimes (|0\rangle_{\text{gs}} \langle 0|_{\text{gs}}) . \quad (3.24)$$

If we write $\tilde{\rho}$ in diagonal form,

$$\tilde{\rho} = \sum_{\alpha} P_{\alpha} |\tilde{\alpha}\rangle \langle \tilde{\alpha}|, \quad (3.25)$$

then

$$\rho = \sum_{\alpha} P_{\alpha} |\tilde{\alpha} \otimes 0_{\text{gs}}\rangle \langle \tilde{\alpha} \otimes 0_{\text{gs}}|. \quad (3.26)$$

The entropy is

$$S = -\text{Tr} \rho \ln \rho = -\sum_{\alpha} s(P_{\alpha}) = -\text{Tr} \tilde{\rho} \ln \tilde{\rho}. \quad (3.27)$$

Since any vacuum-bounded ρ has this form, a variation of ρ that preserves the constraints must also have this form,

$$\delta\rho = \tilde{\delta\rho} \otimes (|0\rangle_{\text{gs}} \langle 0|_{\text{gs}}). \quad (3.28)$$

If $S = -\text{Tr}(\rho + t\delta\rho) \ln(\rho + t\delta\rho) = -\text{Tr}(\tilde{\rho} + t\tilde{\delta\rho}) \ln(\tilde{\rho} + t\tilde{\delta\rho})$, then

$$\frac{dS}{dt} = -\text{Tr} \tilde{\delta\rho} \ln \tilde{\rho}. \quad (3.29)$$

If ρ maximizes S subject to the constraints, then we must have $\text{Tr} \tilde{\delta\rho} \ln \tilde{\rho}$ for any variation $\tilde{\delta\rho}$ that preserves the constraints, i.e. for which $\text{Tr} \tilde{\delta\rho} = 0$ and

$$\text{Tr} \delta\rho H = \text{Tr} \delta\rho x_i x_j = \text{Tr} \delta\rho P_i P_j = 0. \quad (3.30)$$

Now for any A , $\text{Tr} \delta\rho A = \text{Tr}(\tilde{\delta\rho} \otimes (|0_{\text{gs}}\rangle \langle 0_{\text{gs}}|))A$. When we take the trace we only need to sum over states of the form $|\tilde{\alpha} \otimes 0_{\text{gs}}\rangle$. Thus

$$\langle A \rangle = \text{Tr} \delta\rho A = \sum_{\tilde{\alpha}\tilde{\beta}} \langle \tilde{\alpha} | \tilde{\delta\rho} | \tilde{\beta} \rangle \langle \tilde{\beta} \otimes 0_{\text{gs}} | A | \tilde{\alpha} \otimes 0_{\text{gs}} \rangle = \text{Tr} \tilde{\delta\rho} \tilde{A} = \langle \tilde{A} \rangle. \quad (3.31)$$

Thus we are looking for $\tilde{\rho}$ that maximizes $S = -\text{Tr} \tilde{\rho} \ln \tilde{\rho}$ subject to the constraints $\text{Tr} \tilde{\delta\rho} \tilde{H} = \text{Tr} \tilde{\delta\rho} \tilde{x_i x_j} = \text{Tr} \tilde{\delta\rho} \tilde{P_i P_j} = 0$, where i and j range over the outside oscillators. There is no longer a problem of zero eigenvalues of $\tilde{\rho}$.

From Eq. (2.66) we expect $\tilde{\rho}$ to have the form

$$\tilde{\rho} \propto e^{-\beta(\tilde{H} + f_{ij} \tilde{x_i x_j} + g_{ij} \tilde{P_i P_j})}. \quad (3.32)$$

We can write this in a more familiar way as

$$\rho \propto e^{-\beta H'}, \quad (3.33)$$

where H' is a fictitious Hamiltonian for these oscillators,

$$H' = \tilde{H} + f_{ij} \tilde{x_i x_j} + g_{ij} \tilde{P_i P_j}. \quad (3.34)$$

3.2.4 New coordinates

We would now like to introduce new coordinates \mathbf{w} as follows: The first N_{in} \mathbf{w} coordinates will be the inside oscillator coordinates, $\mathbf{w}_{\text{in}} = \mathbf{x}_{\text{in}}$. The last N_{gs} coordinates are the ground state normal modes, $\mathbf{w}_{\text{gs}} = \mathbf{y}_{\text{gs}}$. The remaining N_{in} coordinates can be any coordinates that are independent of those specified so far; we will make a particular choice later.

To do this, we proceed as follows: From Eqs. (3.22) and (3.23) we have

$$YY^{-1} = \left(\begin{array}{c|c} Y_{\text{in},\text{free}} Y_{\text{free,in}}^{-1} & Y_{\text{in},\text{free}} Y_{\text{free,out}}^{-1} \\ \hline Y_{\text{out},\text{free}} Y_{\text{free,in}}^{-1} & Y_{\text{out},\text{free}} Y_{\text{free,out}}^{-1} + Y_{\text{out},\text{gs}} Y_{\text{gs,out}}^{-1} \end{array} \right) = \left(\begin{array}{c|c} N_{\text{in}} & N_{\text{out}} \\ \hline I & 0 \\ 0 & I \end{array} \right) \}_{N_{\text{in}}} \}_{N_{\text{out}}} \quad (3.35)$$

and

$$Y^{-1}Y = \left(\begin{array}{c|c} Y_{\text{free,in}}^{-1} Y_{\text{in},\text{free}} + Y_{\text{free,out}}^{-1} Y_{\text{out},\text{free}} & Y_{\text{free,out}}^{-1} Y_{\text{out,gs}} \\ \hline Y_{\text{gs,out}}^{-1} Y_{\text{out,free}} & Y_{\text{gs,out}}^{-1} Y_{\text{out,gs}} \end{array} \right) = \left(\begin{array}{c|c} N_{\text{free}} & N_{\text{gs}} \\ \hline I & 0 \\ 0 & I \end{array} \right) \}_{N_{\text{free}}} \}_{N_{\text{gs}}} \quad (3.36)$$

In particular, $Y_{\text{gs,out}}^{-1} Y_{\text{out,gs}} = I$. We would like to extend $Y_{\text{gs,out}}^{-1}$ and $Y_{\text{out,gs}}$ into square matrices R and R^{-1} with

$$R = \left(\begin{array}{c|c} N_{\text{in}} & N_{\text{gs}} \\ \hline D & Y_{\text{out,gs}} \end{array} \right) \}_{N_{\text{out}}} \quad (3.37)$$

and

$$R^{-1} = \left(\begin{array}{c} N_{\text{out}} \\ \hline \frac{D'}{Y_{\text{gs,out}}^{-1}} \end{array} \right) \}_{N_{\text{in}}} \quad (3.38)$$

This means that we must find D and D' such that

$$Y_{\text{gs,out}}^{-1} D = 0 \quad (3.39a)$$

$$D' Y_{\text{out,gs}} = 0 \quad (3.39b)$$

$$D'D = I. \quad (3.39c)$$

There are many possible choices of D and D' that satisfy Eqs. (3.39). Here we proceed as follows: Let

$$Z = \left(\begin{array}{c} Z_{\text{in}} \\ \hline Z_{\text{out}} \end{array} \right) \quad (3.40a)$$

$$Z^{-1} = (Z_{\text{in}}^{-1} | Z_{\text{out}}^{-1}) \quad (3.40b)$$

so that $Z_{\text{in}}Z_{\text{in}}^{-1} = I$, $Z_{\text{out}}Z_{\text{out}}^{-1} = I$ and $Z_{\text{in}}^{-1}Z_{\text{in}} + Z_{\text{out}}^{-1}Z_{\text{out}} = I$. Now let

$$\bar{D} = \frac{1}{2}Z_{\text{out}}Z_{\text{in}}^T = \langle 0|\mathbb{X}|0\rangle_{\text{out,in}} \quad (3.41\text{a})$$

$$\bar{D}' = \frac{1}{2}Z_{\text{in}}^{-1T}Z_{\text{out}}^{-1} = \langle 0|\mathbb{P}|0\rangle_{\text{in,out}}, \quad (3.41\text{b})$$

let A and B be $N_{\text{in}} \times N_{\text{in}}$ matrices with

$$AB = (\bar{D}'\bar{D})^{-1} \quad (3.42)$$

and let

$$D = \bar{D}A \quad (3.43\text{a})$$

$$D' = B\bar{D}' . \quad (3.43\text{b})$$

We also divide

$$W = \left(\begin{array}{c|c} W_{\text{free}} & W_{\text{gs}} \end{array} \right) . \quad (3.44)$$

Since $Y = ZW$ and $Y^{-1} = W^T Z^{-1}$, we have

$$Z_{\text{in}}W_{\text{gs}} = 0 \quad (3.45\text{a})$$

$$W_{\text{gs}}^T Z_{\text{in}}^{-1} = 0 . \quad (3.45\text{b})$$

Thus

$$D'Y_{\text{out,gs}} \propto BZ_{\text{in}}^{-1T}Z_{\text{out}}^{-1}Z_{\text{out}}W_{\text{gs}} = BZ_{\text{in}}^{-1T}W_{\text{gs}} - BZ_{\text{in}}^{-1T}Z_{\text{in}}W_{\text{gs}} = 0 \quad (3.46)$$

by Eqs. (3.45) and their transposes. Similarly

$$Y_{\text{gs,out}}^{-1}D \propto W_{\text{gs}}^T Z_{\text{out}}^{-1}Z_{\text{out}}Z_{\text{in}}^TA = W_{\text{gs}}^T Z_{\text{in}}^TA - W_{\text{gs}}^T Z_{\text{in}}^{-1}Z_{\text{in}}Z_{\text{in}}^TA = 0 . \quad (3.47)$$

From Eq. (3.42) we find $D'D = I$. Thus the matrices D and D' satisfy Eqs. (3.39). We still have the freedom of choosing the matrix A arbitrarily.

Now let

$$Q = \left(\begin{array}{c|c} \begin{array}{c} N_{\text{in}} \\ \hline I \end{array} & \begin{array}{c} N_{\text{out}} \\ 0 \end{array} \\ \hline 0 & R \end{array} \right) \}^{N_{\text{in}}} \}^{N_{\text{out}}} \quad (3.48)$$

and define \mathbf{w} by $\mathbf{x} = Q\mathbf{w}$ so $\mathbf{P}_x = Q^{-1T}\mathbf{P}_w$. Then $\mathbf{w}_{\text{in}} = \mathbf{x}_{\text{in}}$ and $\mathbf{w}_{\text{gs}} = \mathbf{y}_{\text{gs}}$ as desired.

3.2.5 Reduced operators

We would like to recast our problem in terms of \mathbf{w}_{free} , the the first N_{free} \mathbf{w} coordinates. First we look at the operators $x_\mu x_\nu = \mathbb{X}_{\mu\nu}$ and $P_\mu P_\nu = \mathbb{P}_{\mu\nu}$. If we write

$$Q = (Q_{\text{free}} | Q_{\text{gs}}) \quad (3.49\text{a})$$

$$Q^{-1} = \begin{pmatrix} Q_{\text{free}}^{-1} \\ Q_{\text{gs}}^{-1} \end{pmatrix}, \quad (3.49\text{b})$$

we have $\mathbf{x} = Q\mathbf{w} = Q_{\text{free}}\mathbf{w}_{\text{free}} + Q_{\text{gs}}\mathbf{w}_{\text{gs}}$ and $\mathbf{P} = Q^{-1T}\mathbf{P}_w = Q_{\text{free}}^{-1T}(\mathbf{P}_w)_{\text{free}} + Q_{\text{gs}}^{-1}(\mathbf{P}_w)_{\text{gs}}$, so

$$\mathbb{X} = Q_{\text{free}}\mathbb{W}_{\text{free},\text{free}}Q_{\text{free}}^T + Q_{\text{gs}}\mathbb{W}_{\text{gs},\text{gs}}Q_{\text{gs}}^T \quad (3.50\text{a})$$

$$\mathbb{P} = Q_{\text{free}}^{-1T}(\mathbb{P}_w)_{\text{free},\text{free}}Q_{\text{free}}^{-1} + Q_{\text{gs}}^{-1T}(\mathbb{P}_w)_{\text{gs},\text{gs}}Q_{\text{gs}}^{-1}. \quad (3.50\text{b})$$

Now we form the reduced operators $\widetilde{x_\mu x_\nu}$ and $\widetilde{P_\mu P_\nu}$. Since $\mathbf{w}_{\text{gs}} = \mathbf{y}_{\text{gs}}$ and the \mathbf{y}_{gs} modes are in the ground state by definition, $\widetilde{\mathbb{W}}_{\text{gs},\text{gs}} = (\widetilde{\mathbb{P}_w})_{\text{gs},\text{gs}} = (1/2)I$, and so

$$\widetilde{\mathbb{X}} = Q_{\text{free}}\mathbb{W}_{\text{free},\text{free}}Q_{\text{free}}^T + \frac{1}{2}Q_{\text{gs}}Q_{\text{gs}}^T \quad (3.51\text{a})$$

$$\widetilde{\mathbb{P}} = Q_{\text{free}}^{-1T}(\mathbb{P}_w)_{\text{free},\text{free}}Q_{\text{free}}^{-1} + \frac{1}{2}Q_{\text{gs}}^{-1T}Q_{\text{gs}}^{-1}. \quad (3.51\text{b})$$

In each case the second term is just a constant. Now

$$H = \frac{1}{2}(P_\mu P_\mu + K_{\mu\nu}x_\mu x_\nu) = \frac{1}{2}\text{Tr}(\mathbb{P} + K\mathbb{X}) \quad (3.52)$$

where the trace is over the oscillator indices. Thus

$$\begin{aligned} \tilde{H} &= \frac{1}{2}\text{Tr}\left(Q_{\text{free}}^{-1T}(\mathbb{P}_w)_{\text{free},\text{free}}Q_{\text{free}}^{-1} + KQ_{\text{free}}\mathbb{W}_{\text{free},\text{free}}Q_{\text{free}}^T\right) + \text{const} \\ &= \frac{1}{2}\text{Tr}\left(\tilde{T}(\mathbb{P}_w)_{\text{free},\text{free}} + \tilde{K}\mathbb{W}_{\text{free},\text{free}}\right) + \text{const} \end{aligned} \quad (3.53)$$

where

$$\tilde{T} = Q_{\text{free}}^{-1}Q_{\text{free}}^{-1T} = \left(\begin{array}{c|c} I & 0 \\ \hline 0 & D'D'^T \end{array}\right)_{N_{\text{in}}}^{N_{\text{in}}} \quad (3.54\text{a})$$

$$\tilde{K} = Q_{\text{free}}^T K Q_{\text{free}} = \left(\begin{array}{c|c} K_{\text{in,in}} & K_{\text{in,out}}D \\ \hline D^T K_{\text{out,in}} & D^T K_{\text{out,out}}D \end{array}\right)_{N_{\text{in}}}^{N_{\text{in}}}. \quad (3.54\text{b})$$

The constant term in Eq. (3.53) is

$$\frac{1}{2}\text{Tr}\left(KQ_{\text{gs}}Q_{\text{gs}}^T + Q_{\text{gs}}^{-1T}Q_{\text{gs}}^{-1}\right) = \frac{1}{2}\text{Tr}\left(Y_{\text{out,gs}}^T K_{\text{out,out}} Y_{\text{out,gs}} + Y_{\text{gs,out}}^{-1T} Y_{\text{gs,out}}^{-1}\right). \quad (3.55)$$

It depends on the ground state modes only and is just part of the zero-point energy. It will be the same in the vacuum and in a vacuum-bounded state. Thus if instead

of Eq. (3.53) we use

$$\tilde{H} = \frac{1}{2} \text{Tr} \left(\tilde{T}(\mathbb{P}_w)_{\text{free,free}} + \tilde{K} \mathbb{W}_{\text{free,free}} \right) \quad (3.56)$$

we are just shifting \tilde{H} by a constant term and thus changing the zero-point energy.

Now we would like to make this reduced system look as much as possible like the system we started with. Let B_1 be some matrix such that $B_1^T B_1 = (\bar{D}' \bar{D}'^T)^{-1}$, let B_2 be a unitary matrix to be determined, and let $B = B_2 B_1$. Then $D' D'^T = I$, so $\tilde{T} = I$. This gives $A = A_1 A_2$ where $A_1 = (\bar{D}' \bar{D})^{-1} B_1^{-1}$ and $A_2 = B_2^T$. Let $D_1 = \bar{D} A_1$ and let

$$\tilde{K}_1 = \left(\begin{array}{c|c} K_{\text{in,in}} & K_{\text{in,out}} D_1 \\ \hline D_1^T K_{\text{out,in}} & D_1^T K_{\text{out,out}} D_1 \end{array} \right). \quad (3.57)$$

Now

$$K_{\text{in,out}} = \begin{pmatrix} & 0 \\ \hline -g & \end{pmatrix}, \quad (3.58)$$

so $K_{\text{in,out}} D_1$ is nonzero only in the last row. Thus the last $N_{\text{in}} + 1$ rows and columns of \tilde{K}_1 look like

$$\left(\begin{array}{c|c} 1 & N_{\text{in}} \\ \hline 2g & ? \\ \hline ? & ? \end{array} \right) \}^1_{N_{\text{in}}}. \quad (3.59)$$

A matrix of size $(N_{\text{in}} + 1) \times (N_{\text{in}} + 1)$ can be put in tridiagonal form by a unitary transform of the form

$$\left(\begin{array}{c|c} 1 & N_{\text{in}} \\ \hline 1 & 0 \\ \hline 0 & U \end{array} \right) \}^1_{N_{\text{in}}} \quad (3.60)$$

which can be constructed using the Householder process. (See, e.g., [36] section 11.2.) We will use this to choose $A_1 = U$, so that \tilde{K} will be tridiagonal. For each off-diagonal element in the resulting tridiagonal matrix there is a choice of sign, and we will choose them all to be negative. Thus in the \mathbf{w} coordinates, each oscillator has unit mass and is coupled only to its neighbors. This completely specifies the matrices A and B and thus D and D' . Note that D and D' do not depend on the undetermined parts of W .

To make H' in Eq. (3.34) we can add to \tilde{H} a kinetic and potential term involving outside oscillators only. The potential term (disregarding a constant) is

$$f_{ij} \tilde{x}_i \tilde{x}_j = \text{Tr} f \tilde{\mathbb{X}}_{\text{out,out}} = \text{Tr} f Q_{\text{out,free}} \mathbb{W}_{\text{free,free}} Q_{\text{out,free}}^T. \quad (3.61)$$

Since

$$Q_{\text{out,free}} = \left(\begin{array}{c|c} & N_{\text{in}} \\ \hline 0 & D \end{array} \right) \}_{N_{\text{out}}}, \quad (3.62)$$

this term is equivalent to adding an arbitrary term to just the lower right part of \tilde{K} .

Similarly the kinetic term is

$$g_{ij} \widetilde{P_i P_j} = \text{Tr } g \widetilde{\mathbb{P}}_{\text{out,out}} = \text{Tr } g Q_{\text{free,out}}^{-1T} (\mathbb{P}_w)_{\text{free,free}} Q_{\text{free,out}}^{-1}. \quad (3.63)$$

Since

$$Q_{\text{free,out}}^{-1} = \left(\begin{array}{c|c} 0 & N_{\text{out}} \\ \hline D' & \} N_{\text{in}} \end{array} \right), \quad (3.64)$$

this term corresponds to adding an arbitrary term to just the lower right part of \tilde{T} .

That is to say we can write

$$H' = \frac{1}{2} \text{Tr } (T' (\mathbb{P}_w)_{\text{free,free}} + K' \mathbb{W}_{\text{free,free}}) \quad (3.65)$$

with

$$T' = \left(\begin{array}{c|c} I & 0 \\ \hline 0 & ? \end{array} \right) \quad (3.66a)$$

$$K' = \left(\begin{array}{c|c} K_{\text{in,in}} & K_{\text{in,out}} D \\ \hline D^T K_{\text{out,in}} & ? \end{array} \right). \quad (3.66b)$$

3.2.6 Reduced constraints

Now we rewrite our constraints, Eqs. (3.9), in terms of the \mathbf{w} coordinates. We will keep only the parts of the constraint equations that are not automatically satisfied because of the ground-state modes. For the expectation value constraints, from Eqs. (3.31) and (3.51) we have

$$\begin{aligned} \langle \mathbb{X} \rangle_{\text{out,out}} &= \langle \widetilde{\mathbb{X}} \rangle_{\text{out,out}} = Q_{\text{out,free}} \langle \mathbb{W} \rangle_{\text{free,free}} Q_{\text{out,free}}^T + \frac{1}{2} Q_{\text{out,gs}} Q_{\text{out,gs}}^T \\ &= D \langle \mathbb{W} \rangle_{\text{mid,mid}} D^T + \text{const} \end{aligned} \quad (3.67a)$$

$$\begin{aligned} \langle \mathbb{P} \rangle_{\text{out,out}} &= \langle \widetilde{\mathbb{P}} \rangle_{\text{out,out}} = Q_{\text{free,out}}^{-1T} \langle \mathbb{P}_w \rangle_{\text{free,free}} Q_{\text{free,out}}^{-1} + \frac{1}{2} Q_{\text{gs,out}}^{-1T} Q_{\text{gs,out}}^{-1} \\ &= D'^T \langle \mathbb{P}_w \rangle_{\text{mid,mid}} D' + \text{const} \end{aligned} \quad (3.67b)$$

where \mathbf{w}_{mid} means the outside elements of \mathbf{w}_{free} , i.e. $w_{N_{\text{in}}+1} \dots w_{2N_{\text{in}}}$.

These expectation value matrices must be the same in the vacuum as in the vacuum-bounded state. We can accomplish this by requiring that $\langle \mathbb{P}_w \rangle_{\text{mid,mid}}$ and $\langle \mathbb{W} \rangle_{\text{mid,mid}}$ are the same as in the vacuum. Thus we have reduced the problem to one that has only $N_{\text{in}}(N_{\text{in}} + 1)$ expectation value constraints, regardless of the value of N_{out} .

For the energy constraint, Eq. (3.9a), we are concerned only with the renormalized energy $\text{Tr } \rho H - \langle 0 | H | 0 \rangle$. Thus the constant term in Eq. (3.53) does not contribute, and we can use \tilde{H} from Eq. (3.56). Once again there is no dependence on N_{out} .

3.2.7 Derivation based on inside functions

We would now like to redo the proceeding calculation in a way which does not depend on the number of outside oscillators. Then we can remove the box from our system by taking $L \rightarrow \infty$ and $N \rightarrow \infty$. It appears that we have used the matrices D and D' which have an index that runs from 1 to N_{out} . However, we have used them only in particular combinations. The quantities which we need in our calculation are

1. $K_{\text{in,out}}\bar{D}$
2. $\bar{D}'\bar{D}$
3. $\bar{D}'\bar{D}'^T$
4. $\bar{D}^T K_{\text{out,out}}\bar{D}$.

Each of these quantities is an $N_{\text{in}} \times N_{\text{in}}$ matrix, so it is reasonable to imagine that they do not depend on N_{out} in the $N \rightarrow \infty$ limit.

We proceed as follows: From Eqs. (3.41) we have

$$\bar{D} = \langle \mathbb{X} \rangle_{\text{out,in}} \quad (3.68a)$$

$$\bar{D}' = \langle \mathbb{P} \rangle_{\text{in,out}}. \quad (3.68b)$$

Any given element of $\langle \mathbb{X} \rangle$ and $\langle \mathbb{P} \rangle$ has a smooth limit when N_{out} is taken to infinity. It is just a particular expectation value of a half-line of coupled oscillators, which is a well-defined problem. We can express the above items in terms of such elements as follows:

1. $K_{\text{in,out}}\bar{D}$ depends only on the first row of \bar{D} which is $\langle \mathbb{X} \rangle_{N_{\text{in}}+1,\text{in}}$ so it is already well-defined in the limit.
2. From Eq. (3.16b) we have

$$\langle \mathbb{P} \rangle \langle \mathbb{X} \rangle = \frac{1}{4}I \quad (3.69)$$

so $\bar{D}'\bar{D} = \langle \mathbb{P} \rangle_{\text{in,out}}\langle \mathbb{X} \rangle_{\text{out,in}} = \frac{1}{4}I - \langle \mathbb{P} \rangle_{\text{in,in}}\langle \mathbb{X} \rangle_{\text{in,in}}$, which does not depend on N_{out} .

3. We expand $\langle \mathbb{P} \rangle \langle \mathbb{P} \rangle = \frac{1}{4}Z^{-1}Z^{-1}Z^{-1}Z^{-1}$. We insert $I = Z\Omega_0Z^T$ here to get

$$\langle \mathbb{P} \rangle \langle \mathbb{P} \rangle = \frac{1}{4}Z^{-1}Z^{-1}\Omega_0Z^{-1} = \frac{1}{4}K. \quad (3.70)$$

Then $\bar{D}'\bar{D}'^T = \langle \mathbb{P} \rangle_{\text{in,out}}\langle \mathbb{P} \rangle_{\text{out,in}} = \frac{1}{4}K_{\text{in,in}} - \langle \mathbb{P} \rangle_{\text{in,in}}\langle \mathbb{P} \rangle_{\text{in,in}}$ which does not depend on N_{out} .

4. Using Eqs. (3.69) and (3.70) we can write

$$\langle \mathbb{X} \rangle K = K \langle \mathbb{X} \rangle = \langle \mathbb{P} \rangle \quad \text{and} \quad \langle \mathbb{X} \rangle K \langle \mathbb{X} \rangle = \frac{1}{4}I \quad (3.71)$$

so

$$\begin{aligned} \frac{1}{4}I &= \langle \mathbb{X} \rangle_{\text{in,out}} K_{\text{out,out}} \langle \mathbb{X} \rangle_{\text{out,in}} + \langle \mathbb{X} \rangle_{\text{in,in}} K_{\text{in,out}} \langle \mathbb{X} \rangle_{\text{out,in}} \\ &\quad + \langle \mathbb{X} \rangle_{\text{in,out}} K_{\text{out,in}} \langle \mathbb{X} \rangle_{\text{in,in}} + \langle \mathbb{X} \rangle_{\text{in,in}} K_{\text{in,in}} \langle \mathbb{X} \rangle_{\text{in,in}} \\ &= \bar{D}^T K_{\text{out,out}} \bar{D} + \langle \mathbb{X} \rangle_{\text{in,in}} (\langle \mathbb{P} \rangle_{\text{in,in}} - K_{\text{in,in}} \langle \mathbb{X} \rangle_{\text{in,in}}) \\ &\quad + (\langle \mathbb{P} \rangle_{\text{in,in}} - \langle \mathbb{X} \rangle_{\text{in,in}} K_{\text{in,in}}) \langle \mathbb{X} \rangle_{\text{in,in}} + \langle \mathbb{X} \rangle_{\text{in,in}} K_{\text{in,in}} \langle \mathbb{X} \rangle_{\text{in,in}} \end{aligned} \quad (3.72)$$

and so

$$\bar{D}^T K_{\text{out,out}} \bar{D} = \frac{1}{4}I - \langle \mathbb{X} \rangle_{\text{in,in}} \langle \mathbb{P} \rangle_{\text{in,in}} - \langle \mathbb{P} \rangle_{\text{in,in}} \langle \mathbb{X} \rangle_{\text{in,in}} + \langle \mathbb{X} \rangle_{\text{in,in}} K_{\text{in,in}} \langle \mathbb{X} \rangle_{\text{in,in}} \quad (3.73)$$

which does not depend on N_{out} .

Thus we can now take $N \rightarrow \infty$ with N_{in} fixed and have a well-defined problem in terms of \tilde{K} with a finite number of free parameters.

3.2.8 Calculation of the reduced vacuum

We are trying to compute \tilde{K} in Eq. (3.54b) in the $N_{\text{out}} \rightarrow \infty$ limit. We will keep N_{in} and the oscillator spacing $L_1 \equiv L/(N+1)$ fixed. With the normalization in Eq. (3.12) the vacuum normal mode matrix is given by

$$Z_{\mu\nu} = \sqrt{\frac{2}{N+1}} \frac{\sin k_{\nu}\mu}{\sqrt{\omega_{\nu}}} \quad (3.74)$$

with

$$k_{\nu} = \frac{\pi\nu}{N+1} \quad (3.75)$$

and

$$\omega_{\nu} = \frac{2(N+1)}{L} \sin \frac{k_{\nu}}{2} = \frac{2}{L_1} \sin \frac{k_{\nu}}{2}. \quad (3.76)$$

Thus

$$\begin{aligned} \langle \mathbb{X} \rangle_{\mu\nu} &= \frac{1}{2} (ZZ^T)_{\mu\nu} = \frac{1}{N+1} \sum_{\alpha=1}^N \frac{\sin k_{\alpha}\mu \sin k_{\alpha}\nu}{\omega_{\alpha}} \\ &= \frac{L_1}{2(N+1)} \sum_{\alpha=1}^N \frac{\sin k_{\alpha}\mu \sin k_{\alpha}\nu}{\sin(k_{\alpha}/2)}. \end{aligned} \quad (3.77)$$

Now we use

$$\cos(\theta - \phi) - \cos(\theta + \phi) = 2 \sin \theta \sin \phi \quad (3.78)$$

to write

$$\langle \mathbb{X} \rangle_{\mu\nu} = \frac{L_1}{4(N+1)} \sum_{\alpha=1}^N \frac{\cos k_{\alpha}(\mu - \nu) - \cos k_{\alpha}(\mu + \nu)}{\sin(k_{\alpha}/2)}. \quad (3.79)$$

Using Eq. (3.78) again, for any number a we can write

$$\frac{\cos k_\alpha(a-1) - \cos k_\alpha a}{\sin(k_\alpha/2)} = 2 \sin k_\alpha(a-1/2) \quad (3.80)$$

and thus

$$\frac{\cos k_\alpha(\mu-\nu) - \cos k_\alpha(\mu+\nu)}{\sin(k_\alpha/2)} = 2 \sum_{a=\mu-\nu+1}^{\mu+\nu} \sin k_\alpha(a-1/2). \quad (3.81)$$

If we put Eq. (3.81) into Eq. (3.79) and bring the sum over α inside the sum over a we get a sum that we can do,

$$2 \sum_{\alpha=1}^N \sin \frac{\pi \alpha(a-1/2)}{N+1} = \cot \frac{\pi(2a-1)}{4(N+1)} + (-1)^a. \quad (3.82)$$

Now we sum this over a . Since $\mu-\nu$ and $\mu+\nu$ have the same parity, the $(-1)^a$ term does not contribute and we get

$$\langle \mathbb{X} \rangle_{\mu\nu} = \frac{L_1}{4(N+1)} \sum_{a=\mu-\nu+1}^{\mu+\nu} \cot \frac{\pi(2a-1)}{4(N+1)}. \quad (3.83)$$

The sum over N has been eliminated. In the $N \rightarrow \infty$ limit, the argument of \cot goes to zero and so we can use $\cot x = 1/x + O(x^{-3})$ to get

$$\langle \mathbb{X} \rangle_{\mu\nu} = \frac{L_1}{\pi} \sum_{a=\mu-\nu+1}^{\mu+\nu} \frac{1}{2a-1}. \quad (3.84)$$

The sum can be done using special functions:

$$\langle \mathbb{X} \rangle_{\mu\nu} = \frac{L_1}{2\pi} \left[\psi \left(\mu + \nu + \frac{1}{2} \right) - \psi \left(\mu - \nu + \frac{1}{2} \right) \right] \quad (3.85)$$

where ψ is the digamma function $\psi(x) = \Gamma'(x)/\Gamma(x)$.

To compute $\langle \mathbb{P} \rangle$ we write the inverse of the normal mode matrix,

$$Z_{\mu\nu}^{-1} = \sqrt{\frac{2\omega_\mu}{N+1}} \sin k_\mu \nu \quad (3.86)$$

and

$$\begin{aligned} \langle \mathbb{P} \rangle_{\mu\nu} &= \frac{1}{2} \left(Z^{-1T} Z^{-1} \right)_{\mu\nu} = \frac{1}{N+1} \sum_{\alpha=1}^N \omega_\alpha \sin k_\alpha \mu \sin k_\alpha \nu \\ &= \frac{2}{L_1(N+1)} \sum_{\alpha=1}^N \sin \frac{k_\alpha}{2} \sin k_\alpha \mu \sin k_\alpha \nu. \end{aligned} \quad (3.87)$$

In this case the sum can be done directly. Using Eq. (3.78) we can write

$$\langle \mathbb{P} \rangle_{\mu\nu} = C_{\mu-\nu} - C_{\mu+\nu} \quad (3.88)$$

where

$$\begin{aligned} C_\lambda &\equiv \frac{1}{L_1(N+1)} \sum_{\alpha=1}^N \sin \frac{k_\alpha}{2} \cos k_\alpha \lambda \\ &= \frac{1}{4L_1(N+1)} \left[\cot \frac{\pi(2\lambda+1)}{4(N+1)} - \cot \frac{\pi(2\lambda-1)}{4(N+1)} - 2(-1)^\lambda \right]. \end{aligned} \quad (3.89)$$

Again we take $N \gg \lambda$ to get

$$C_\lambda = \frac{1}{\pi L_1} \left(\frac{1}{2\lambda+1} - \frac{1}{2\lambda-1} \right) = -\frac{2}{\pi L_1 (4\lambda^2 - 1)} \quad (3.90)$$

and

$$\langle \mathbb{P} \rangle_{\mu\nu} = \frac{2}{\pi L_1} \left(\frac{1}{4(\mu+\nu)^2 - 1} - \frac{1}{4(\mu-\nu)^2 - 1} \right). \quad (3.91)$$

Equations (3.85) and (3.91) give $\langle \mathbb{X} \rangle$ and $\langle \mathbb{P} \rangle$ in the $N_{\text{out}} \rightarrow \infty$ limit. Using these values in the procedure of sections 3.2.4 through 3.2.7 we can compute the matrix \tilde{K} numerically for a system with inside length L_{in} but no outside box.

3.3 Calculation of the vacuum-bounded state

Once we have computed \tilde{K} we can go on to look for a vacuum-bounded state. We are working entirely with the reduced coordinates. With

$$\rho \propto e^{-\beta H'} \quad (3.92)$$

and H' as in Eqs. (3.65–3.66) we have one number, β , and two symmetric $N_{\text{in}} \times N_{\text{in}}$ matrices, $K'_{\text{mid,mid}}$ and $T'_{\text{mid,mid}}$, that we can adjust. The constraints (3.9) involve one scalar constraint, for total energy, and two $N_{\text{in}} \times N_{\text{in}}$ symmetric matrices of constraints, for $w_m w_n$ and $P_{w_m} P_{w_n}$. There are equal numbers of equations to satisfy and free parameters to adjust, and so, if we are lucky, we will be able to find a solution. If we do find a solution, we know it is unique from the arguments of section 2.2.3.

3.3.1 Expectation values

To actually solve these equations we will need to compute the expectation values of $w_m w_n$ and $P_{w_m} P_{w_n}$ given the density matrix (3.92). To do this we find the normal

modes of H' . The Hamiltonian H' gives rise to classical equations of motion

$$\frac{d^2\mathbf{w}_{\text{free}}}{dt^2} = -T'K'\mathbf{w}_{\text{free}}, \quad (3.93)$$

so we look for eigenvectors $\mathbf{w}_{\text{free}}^\alpha$ that satisfy

$$T'K'\mathbf{w}_{\text{free}}^\alpha = \omega_\alpha^2 \mathbf{w}_{\text{free}}^\alpha. \quad (3.94)$$

The eigenvectors will be complete, so that we can define new coordinates u_α via $\mathbf{w}_{\text{free}} = \sum u_\alpha \mathbf{w}_{\text{free}}^\alpha$, which will then obey the equations of motion

$$\frac{d^2u_\alpha}{dt^2} = -\omega_\alpha^2 u_\alpha. \quad (3.95)$$

We can choose the norms of the eigenvectors so that¹ $\mathbf{w}_{\text{free}}^\alpha \cdot K'\mathbf{w}_{\text{free}}^\beta = \omega_\alpha^2 \delta_{\alpha\beta}$ and group the eigenvectors into a matrix U via $U_{\mu\alpha} = w_\mu^\alpha$. Then we will find that $T'_{\mu\nu} = w_\mu^\alpha w_\nu^\alpha$, or

$$K' = U^{-1T} \Omega^2 U^{-1} \quad \text{and} \quad T' = UU^T \quad (3.96)$$

where $\Omega_{\alpha\beta} = \omega_\alpha \delta_{\alpha\beta}$. We can then substitute

$$\mathbf{w}_{\text{free}} = U\mathbf{u} \quad (\mathbf{P}_w)_{\text{free}} = U^{-1T} \mathbf{P}_u \quad (3.97)$$

into H' to get

$$\begin{aligned} H' &= \frac{1}{2} (\mathbf{P}_u \cdot \mathbf{P}_u + \mathbf{u} \cdot \Omega^2 \mathbf{u}) \\ &= \frac{1}{2} \sum_\alpha (P_{u_\alpha}^2 + \omega_\alpha^2 u_\alpha^2) \equiv \sum_\alpha H'_\alpha. \end{aligned} \quad (3.98)$$

This is the Hamiltonian for a set of (fictitious) uncoupled oscillators with frequencies ω_α . The expectation values of the u and P_u are easily computed,

$$\langle u_\alpha u_\beta \rangle = \frac{1}{2\omega_\alpha} \delta_{\alpha\beta} \coth \frac{\beta}{2\omega_\alpha} \quad (3.99a)$$

$$\langle P_{u_\alpha} P_{u_\beta} \rangle = \frac{\omega_\alpha}{2} \delta_{\alpha\beta} \coth \frac{\beta}{2\omega_\alpha} \quad (3.99b)$$

so that in terms of the \mathbf{w} coordinates we have

$$\langle w_m w_n \rangle = \sum_\alpha \frac{1}{2\omega_\alpha} U_{m\alpha} U_{n\alpha} \coth \frac{\beta}{2\omega_\alpha} \quad (3.100a)$$

¹This is a different normalization than we used for Z in section 3.2.1. In the present normalization the original vacuum modes would all have the same amplitude. In section 3.2.1 the modes were multiplied by a factor of $\omega_\alpha^{-1/2}$ relative to the convention here.

$$\langle P_{w_m} P_{w_n} \rangle = \sum_{\alpha} \frac{\omega_{\alpha}}{2} U_{\alpha m}^{-1} U_{\alpha n}^{-1} \coth \frac{\beta}{2} \omega_{\alpha}. \quad (3.100b)$$

In section 4.3 we will compute these expectation values numerically in the vacuum state, given by $H' = \tilde{H}$ and $\beta = \infty$, and require that they have the same values in the vacuum-bounded state with finite β .

3.4 The nature of the results

Before looking at the results of our computations, we would like to learn as much as possible about the form that our answers must take. We will take the frequencies ω_{α} as given here and look at the form of the normal modes \mathbf{w}^{α} .

The vectors $\mathbf{w}_{\text{free}}^{\alpha}$ satisfy the equation

$$T' K' \mathbf{w}_{\text{free}}^{\alpha} = \omega_{\alpha}^2 \mathbf{w}_{\text{free}}^{\alpha} \quad (3.101)$$

with

$$T' = \left(\begin{array}{c|c} I & 0 \\ \hline 0 & T' \end{array} \right) \quad (3.102)$$

and

$$K' = \left(\begin{array}{c|c} K_{\text{in,in}} & K_{\text{in,out}} D \\ \hline D^T K_{\text{out,in}} & K'_{\text{mid,mid}} \end{array} \right). \quad (3.103)$$

However, we have tridiagonalized \tilde{K} , so only the lower left element of $K_{\text{in,out}} D$ is nonzero. In fact, in our numerical work we will find that this element is always $-g$, just as it was in the original $K_{\text{in,out}}$. Thus we have

$$K' = \left(\begin{array}{c|c} K_{\text{in,in}} & 0 \\ \hline -g & K'_{\text{mid,mid}} \\ \hline 0 & \end{array} \right). \quad (3.104)$$

Writing out Eq. (3.101) in components, we get

$$T'_{\mu\nu} K'_{\nu\lambda} w_{\lambda}^{\alpha} = \omega_{\alpha}^2 w_{\mu}^{\alpha}. \quad (3.105)$$

Taking only the inside components of the eigenvalue equation, we see that

$$K'_{a\mu} w_{\mu}^{\alpha} = \omega_{\alpha}^2 w_a^{\alpha} \quad (3.106)$$

for $a \leq N_{\text{in}}$. That is to say,

$$2gw_1^{\alpha} - gw_2^{\alpha} = \omega_{\alpha}^2 w_1^{\alpha} \quad (3.107a)$$

$$-gw_1^{\alpha} + 2gw_2^{\alpha} - gw_3^{\alpha} = \omega_{\alpha}^2 w_2^{\alpha} \quad (3.107b)$$

$$\dots \\ -gw_{N_{\text{in}}-1}^{\alpha} + 2gw_{N_{\text{in}}}^{\alpha} - gw_{N_{\text{in}}+1}^{\alpha} = \omega_{\alpha}^2 w_{N_{\text{in}}}^{\alpha}. \quad (3.107c)$$

Taking ω_{α} fixed, there are N_{in} equations involving $N_{\text{in}} + 1$ unknown components of \mathbf{w}^{α} . However, the equations are invariant under a uniform rescaling of \mathbf{w}^{α} . Thus these N_{in} equations fix w_{μ}^{α} for $\mu = 1 \dots N_{\text{in}} + 1$, except for normalization. The equations are readily solved, and the solution is

$$w_{\mu}^{\alpha} = N'_{\alpha} \sin \mu k'_{\alpha}, \quad (3.108)$$

where

$$\cos k'_{\alpha} = 1 - \frac{\omega_{\alpha}^2}{2g}, \quad (3.109)$$

and N'_{α} is an unknown normalization factor. Here k'_{α} and N'_{α} can be complex, but \mathbf{w}^{α} must be real. When k'_{α} is real we will write $k_{\alpha} = k'_{\alpha}$ and $N_{\alpha} = N'_{\alpha}$ and call this a “normal” mode. When k'_{α} is complex we can write

$$k'_{\alpha} = \pi + ik_{\alpha} \quad (3.110a)$$

$$N'_{\alpha} = iN_{\alpha} \quad (3.110b)$$

$$w_{\mu}^{\alpha} = (-)^{\mu-1} N_{\alpha} \sinh \mu k_{\alpha} \quad (3.110c)$$

with k_{α} and N_{α} real. We will refer to these as “abnormal” modes.

A similar calculation can be done for U^{-1} , the inverse of the eigenvalue matrix U . In this case we will find that

$$U_{\alpha a}^{-1} = N'_{\alpha} \sin ak'_{\alpha}. \quad (3.111)$$

Equation (3.111) has the same form as Eq. (3.108), but applies only for $a = 1 \dots N_{\text{in}}$. That makes Eq. (3.111) less useful than Eq. (3.108) for establishing a connection between the inside and the outside region, and we will not use it further.

Chapter 4

Numerical Solution

Two numerical calculations are necessary to solve the problem. First we must follow the procedure of sections 3.2.4–3.2.8 to find the reduced Hamiltonian \tilde{H} and its vacuum state. Then we must search for parameter values $T'_{\text{mid,mid}}$, $K'_{\text{mid,mid}}$ and β which produce a state with a given energy E_0 but the same expectation values of the outside oscillators.

In fact, we follow a slight variant of the above plan. Instead of fixing E_0 , we hold β fixed. The resulting state has some E_0 and solves the problem of maximizing the entropy for that E_0 , whatever it is. By varying β we can find states for various energies.

In the end we do not use these results directly to calculate bounds on the entropy. Instead we derive a general principle from the numerical calculations, and use this principle as an ansatz to derive a bound in the next chapter.

4.1 Numerical procedures

Finding the reduced vacuum is a fairly straightforward problem in numerical analysis. The number of steps grows as N_{in}^3 . However, in order to produce accurate results for $N_{\text{in}} \gtrsim 6$ it is necessary to use very high-precision floating-point numbers. The necessary number of bits of mantissa in the representation appears to be about $10N_{\text{in}}$.

After finding the reduced vacuum we need to solve a set of simultaneous nonlinear equations. Such problems are in general quite difficult, and require an iterative search for the correct parameter values. Here at least we know from section 2.2.3 that there cannot be more than one solution. Although we have not been able to prove that a solution always exists, in the numerical work we have always been able to find one.

Once the search is sufficiently close to the correct answer it is possible to use Newton's method, which converges quadratically, i.e., the number of correct digits doubles every step. However, the basin of attraction for Newton's method can be quite small and difficult to find. When Newton's method does not work, it is necessary to use some other procedure to make progress toward the solution. Here we used the Powell hybrid method [37,38]. This method moves in a direction which is a combination of the direction Newton's method would suggest and the direction of

steepest descent in the mean square error of the function values. Such a method has the difficulty that it can get stuck at a local minimum of the mean square error that is not a solution. We have been lucky in that there do not seem to be such local minima in this problem.¹

In the case that there are no local minima of the mean square error in the function values, Powell's method is guaranteed to converge from any starting point [37]. However, it often converges quite slowly for large systems, requiring many thousands of iterations to make progress. This has limited our numerical solutions to problems with $N_{\text{in}} \lesssim 15$.

The code was written in Lisp and executed on DECTM AlphaTM workstations. All results presented here were computed using at least 38 decimal digits of precision. The most precise calculation (the reduced vacuum for $N_{\text{in}} = 175$) used 636 digits. The parameters found in Powell's method reproduce the desired expectation values to at least 17 significant digits.

We have made use of many routines from *Numerical Recipes* [2]. However, the code that implements Powell's method was written from scratch in Lisp following the outlines of [37,38] and has many extra features including dynamic increase of working precision as the solution converges.

4.2 Reduction of the vacuum

First we follow the procedures of sections 3.2.4–3.2.8 to calculate the matrix \tilde{K} which gives the ground state of the \mathbf{w}_{free} coordinates. The result is, of course, a tridiagonal matrix which gives a set of self-couplings and nearest-neighbor couplings for the fictitious oscillators \mathbf{w}_{free} . We can express these couplings as multiples of the couplings for a regular chain of N_{free} oscillators with spacing L_1 . Thus we write the self-coupling as

$$\tilde{K}_{\mu\mu} = -gf_{\mu} \quad \left(\sum_{\mu} \right) \quad (4.1)$$

and the nearest-neighbor coupling as

$$\tilde{K}_{\mu,\mu+1} = 2gf_{\mu+1/2} \quad \left(\sum_{\mu} \right) . \quad (4.2)$$

These coupling coefficients converge rapidly to a universal form $f(x)$ where $L_1\mu \rightarrow x$ in the continuum limit. Some results are shown in Fig. 4-1. We can see that $f(x) \approx 1$ until $x \sim 1.4$ at which point it begins to fall and asymptotically approaches 0 as $x \rightarrow 2$. For values of x near 2, $f(x)$ is well fit by

$$f(x) = a(2 - x)^4 \quad (4.3)$$

¹The current formulation of the problem has $O(N_{\text{in}}^2)$ parameters and equations. It is possible to use the normal-mode frequencies and normalizations as our parameters, which gives a problem with only $O(N_{\text{in}})$ parameters and equations. However, this reduction loses the property of having no local minima, and so in fact makes the problem harder to solve.

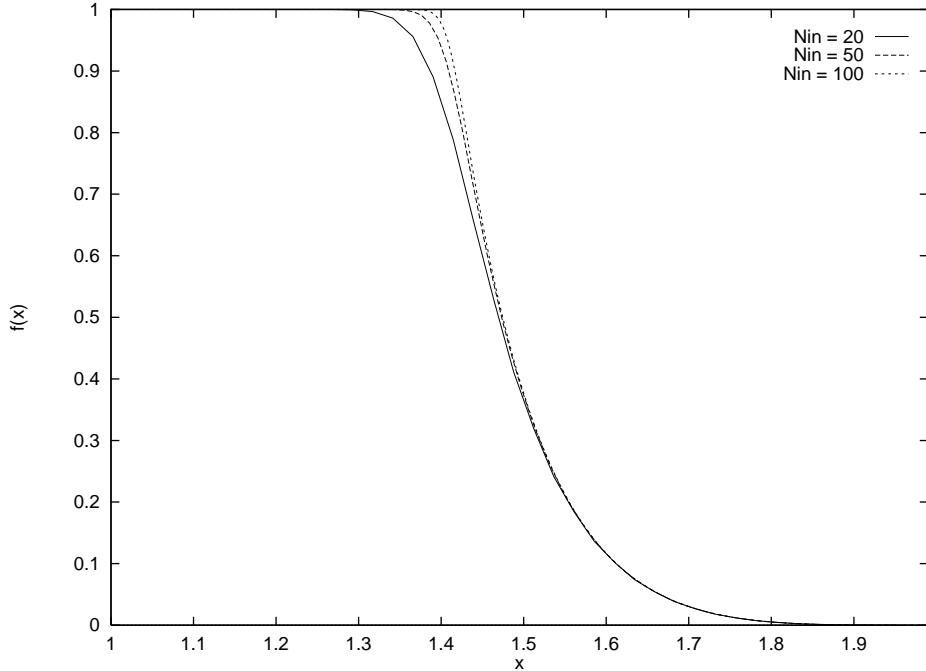


Figure 4-1: The ratio of the coupling coefficients in the reduced problem to what they would be in a regular problem of N_{free} oscillators, plotted against $x = L_1\mu$, for $L_{\text{in}} = 1$.

with $a \approx 3.2$, as shown in Fig. 4-2.

Some typical normal modes of the reduced vacuum are shown in Fig. 4-3. They are sine waves while $f(x) \sim 1$ and then begin to oscillate faster and faster as $f(x)$ shrinks. At first the amplitude of the oscillations grows but for larger x it shrinks rapidly to zero. The wavenumbers in the inside region (and thus the frequencies) are smaller than we would find for a rigid box because most of the oscillations are in the part of the outside region where $f(x) \ll 1$. In fact, as $N_{\text{in}} \rightarrow \infty$ we would expect the low-lying frequencies to go to zero, for the following reason.

We can find the frequencies by computing the normal modes of a Hamiltonian

$$H = \int_0^L dx dy (T(x-y)\pi(x)\pi(y) + K(x-y)\phi(x)\phi(y)) , \quad (4.4)$$

which requires solving the eigenvector equation

$$\int_0^L dy dz T(x-y)K(y-z)g(z) = \lambda g(x) \quad (4.5)$$

with the boundary conditions

$$g(0) = 0 \quad (4.6a)$$

$$g(L) = 0 . \quad (4.6b)$$

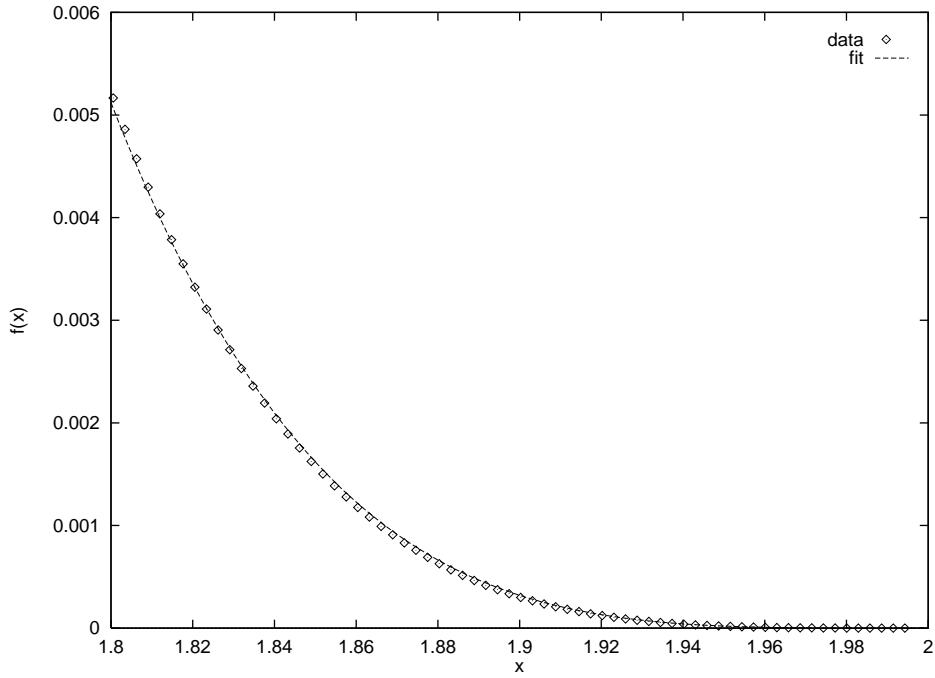


Figure 4-2: The coupling coefficient ratio for $N_{in} = 175$ in the region $x > 1.8$ and the fit $f(x) = 3.2(2 - x)^4$.

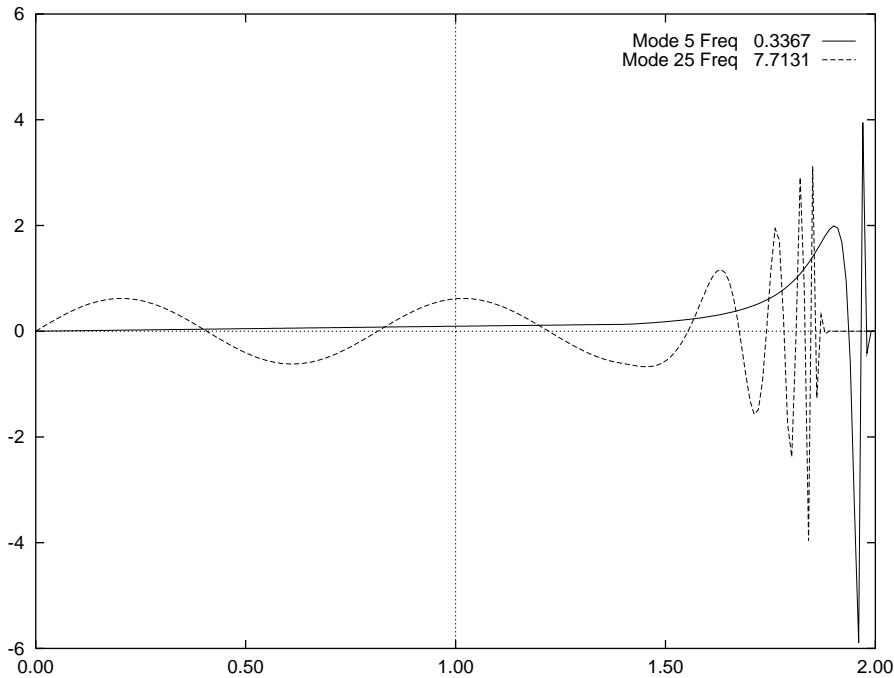


Figure 4-3: The 5th and 25th normal modes in the reduced vacuum, computed with $N_{in} = 175$.

Since Eq. (4.5) is a second-order differential equation we expect two degrees of freedom in the solution. However, one degree of freedom is manifestly the overall scale, which does not affect the boundary conditions. Since there are two boundary conditions but only one free parameter, we can expect to find solutions only for particular values of λ . For example, for the usual scalar field Hamiltonian the general solution to Eq. (4.5) would be

$$g(x) = c \sin(\sqrt{\lambda}x + \delta). \quad (4.7)$$

To satisfy Eqs. (4.6) we need to choose $\delta = 0$ and $\sqrt{\lambda} = n\pi/L$ for some integer n .

However, if we use

$$H = \frac{1}{2} \int_0^{2L_{\text{in}}} f(x) \left[\pi(x)^2 + \left(\frac{d\phi}{dx} \right)^2 \right] dx, \quad (4.8)$$

with $f(x) \rightarrow a(2-x)^4$, as suggested by Fig. 4-2, we will get a continuum of frequencies. The problem is that since $f(x) \rightarrow 0$ as $x \rightarrow 2$ the boundary condition there does not really constrain $g(x)$. There can be arbitrary changes in $g(x)$ near $x = 2$ and so Eq. (4.6b) can always be satisfied. Since there is only one effective boundary condition and one effective degree of freedom, we expect to be able to find a solution for any λ . Thus in the continuum limit there are modes with arbitrarily low frequencies. This is not an unreasonable conclusion, since although the range of x is finite, we are using it to represent the infinite half-line. In the infinite vacuum there is no right-hand boundary condition, and there are modes of every frequency.

This conclusion is confirmed by numerical results. In Fig. 4-4 we plot the lowest normal-mode frequency versus N_{in} . As shown in the figure, the frequencies are well fit by a curve

$$ax^{-1} - x^{-2} \quad (4.9)$$

with $a \approx 1.81$. If this form is correct, in the $N_{\text{in}} \rightarrow \infty$ limit the lowest frequency goes to zero.

If we go to a vacuum-bounded state we will introduce some finite temperature. We then expect that the non-zero temperature will increase the frequencies in such a way that there are only a finite number of low-lying modes and thus a finite entropy. However, in the limit where $T \rightarrow 0$ we do expect an entropy-to-energy relation equivalent to a system with infinitesimal frequencies. This is discussed in the appendix.

4.3 Computation of the vacuum-bounded state

Once we have computed \tilde{K} and the vacuum expectation values of $w_m w_n$ and $P_{w_m} P_{w_n}$, we can proceed to look for the vacuum-bounded state at a particular β . To do this we vary the $N_{\text{in}}(N_{\text{in}} + 1)$ independent components of $T'_{\text{mid,mid}}$ and $K'_{\text{mid,mid}}$ to find those which reproduce the same expectation values of the $N_{\text{in}}(N_{\text{in}} + 1)$ independent operators $w_m w_n$ and $P_{w_m} P_{w_n}$, given in Eqs. (3.100).

To understand the numerical solution we look at the normal mode frequencies

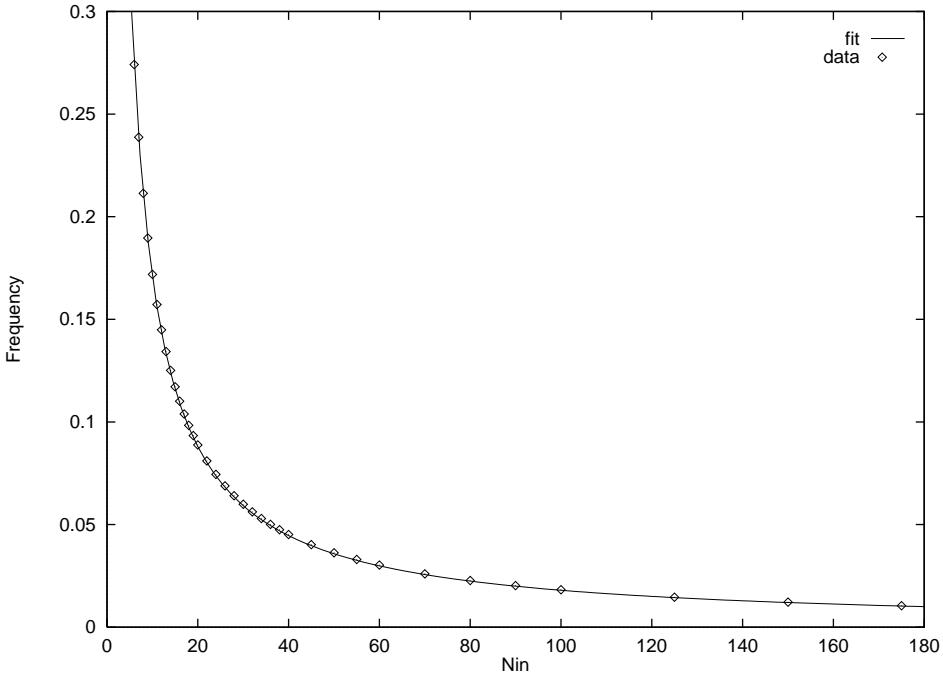


Figure 4-4: The lowest frequency of the reduced vacuum and the fit $1.81x^{-1} - x^{-2}$.

and the forms of the normal modes. When the mode is “normal” (i.e. real k'_α in Eq. (3.108)) there is a sine wave in the inside region. When the mode is “abnormal” there is essentially a growing exponential. Typical modes for a small number of oscillators are shown in Figs. 4-5 and 4-6.

As N becomes large, each “normal” mode and its frequency smoothly approach a limit, providing that we use a normalization appropriate for the continuum, which means that each mode must be rescaled by $L_1^{-1/2}$. In Fig. 4-7 we show the first normal mode for various values of N_{in} . Note that this mode does not appear to come down to zero at $x = 2$. As discussed in section 4.2, this happens because $f(x)$ is going to 0 at $x = 2$ and so there is not really any coupling to the boundary at that point.

As N increases, each abnormal mode and its frequency undergo a smooth evolution, until at some point it disappears from the set of abnormal modes and is replaced by a normal mode with very similar form in the outside region, as shown in Fig. 4-8. Because of this behavior, we believe that if we could solve the continuum behavior directly we would find just the “normal” modes.

4.3.1 Evenly spaced wavenumbers

To address the problem directly for large energies would require numerical solutions for large numbers of oscillators, which is computationally intractable. Instead we would like to extract from the computations in the accessible regime a statement which will allow us to extend our arguments to larger energies. The most striking

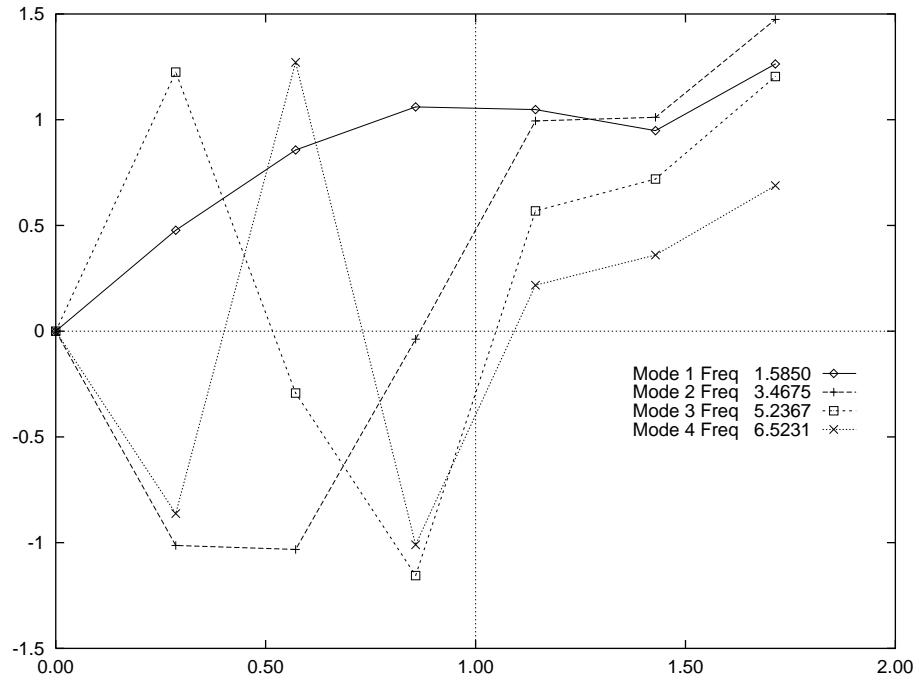


Figure 4-5: Modes and frequencies for the “normal” modes of a system with $L_{in} = 1.0$, $\beta = 2$, $N_{in} = 3$, $N_{free} = 6$.

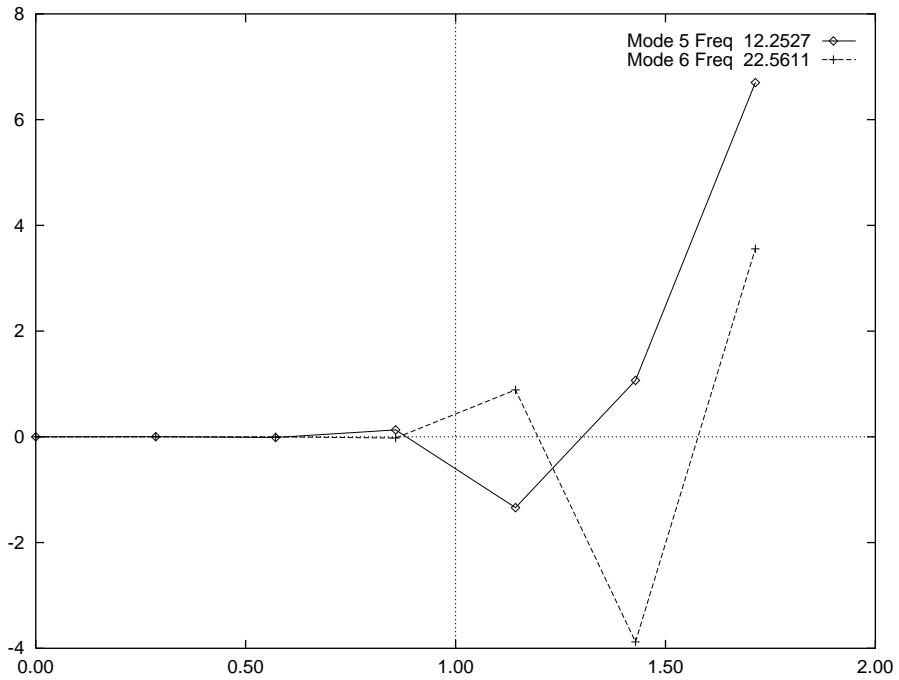


Figure 4-6: Modes and frequencies for the “abnormal” modes of a system with $L_{in} = 1.0$, $\beta = 2$, $N_{in} = 3$, $N_{free} = 6$.

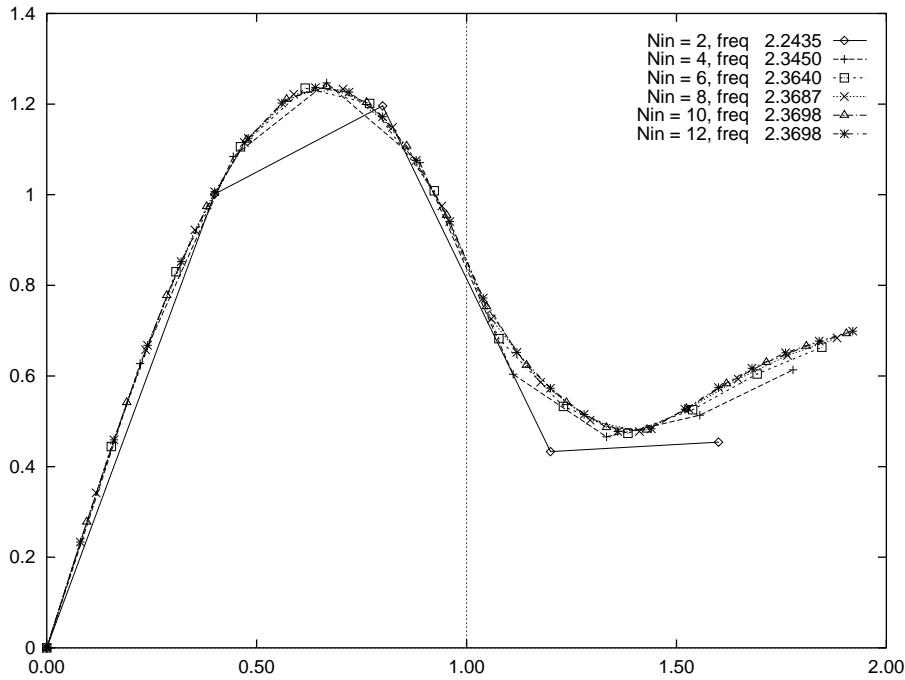


Figure 4-7: The first normal mode, rescaled to the continuum normalization, for various different numbers of oscillators, with $L_{\text{in}} = 1.0$, $\beta = 0.5$.

such result is that the wavenumbers of the “normal” modes are nearly evenly spaced. The larger the energy, the more accurate is this approximation. In Fig. 4-9, we show the wavenumbers for $L_{\text{in}} = 1.0$ and $\beta = 0.5$, which give an energy of about 0.094. Even at this low energy the fit is good to within a few percent of the typical wavenumber. For larger energies the points will lie correspondingly closer to the line.

Since we have set N and L to ∞ , our problem has only two dimensionful parameters, L_{in} and E_0 . Thus there is only one dimensionless parameter, $L_{\text{in}}E_0$, that characterizes the problem. In the 3-dimensional black hole problem the equivalent parameter is RE_0 , which for the parameters in Eq. (1.3) is about 10^{13} . Thus for application to black holes we are interested only in very large values of $L_{\text{in}}E_0$, for which the linear approximation for the “normal” modes will be very good.

Since the “normal” mode wavenumbers extend up to $k \sim \pi$, the number of “normal” modes will be given an integer $N_{\text{norm}} \sim \pi/k_1$ where k_1 is the interval between wavenumbers. In addition there will be $N_{\text{free}} - N_{\text{norm}}$ “abnormal” modes, with frequencies $\omega_\alpha > 2/L_1$. For $N_{\text{in}} \gg L_{\text{in}}/\beta$ these modes do not contribute to the entropy, because they are exponentially suppressed.

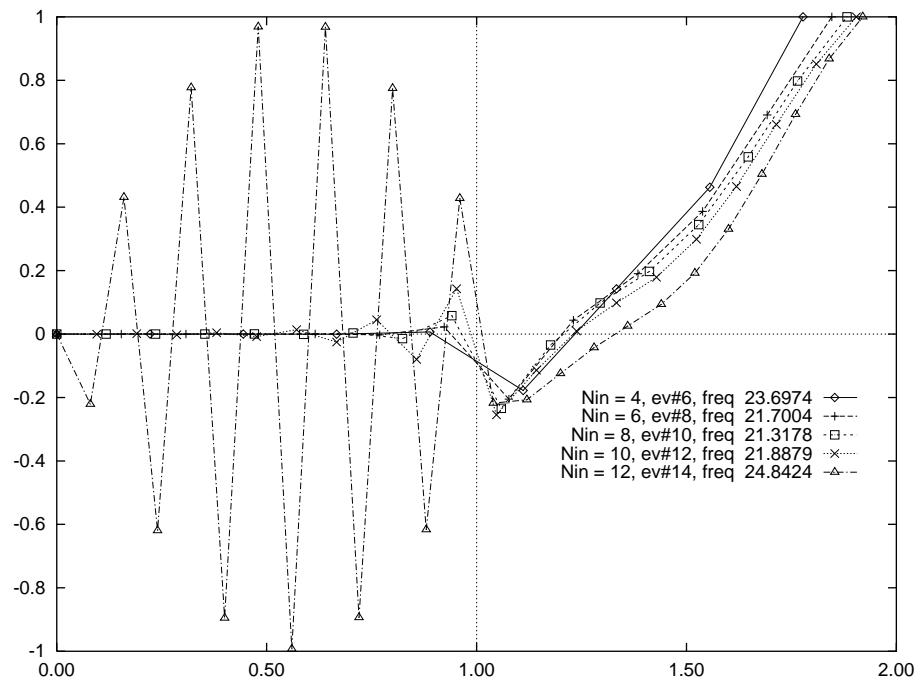


Figure 4-8: An abnormal mode for $L_{in} = 1.0$, $\beta = 0.5$ and various values of N_{in} . The normalizations are chosen to be similar in the outside region. As N_{in} increases the mode changes smoothly until at $N_{in} = 12$ there is no corresponding abnormal mode, but instead one of the new normal modes has a very similar form (but different normalization).

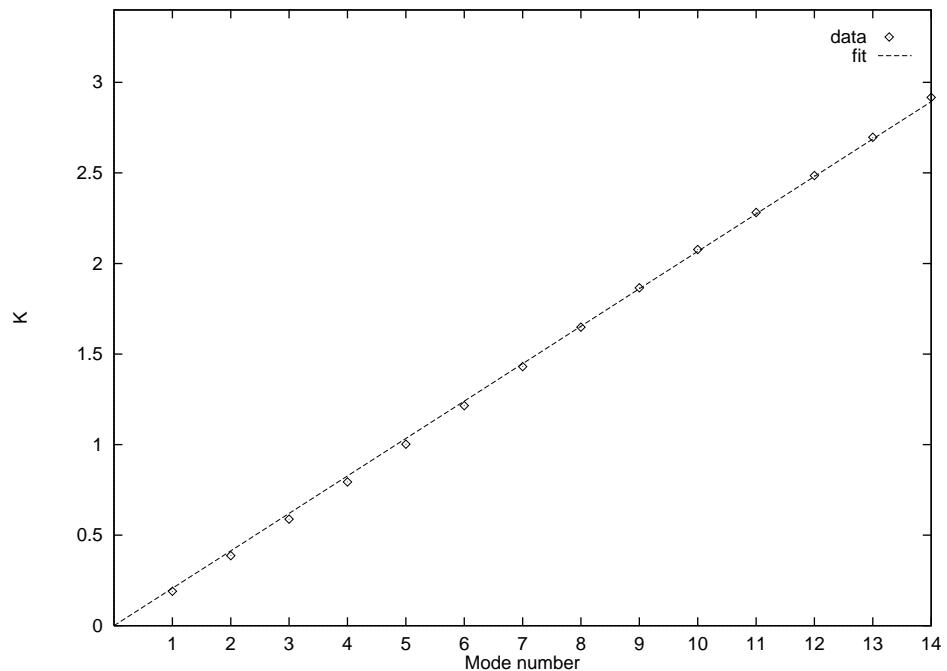


Figure 4-9: The numerically computed wavenumbers compared with the best-fit line through the origin for $L_{in} = 1.0$, $\beta = 0.5$, $N_{in} = 12$.

Chapter 5

The Entropy Bound

As discussed in section 4.3.1, we are interested in vacuum-bounded states for quite large energies. When E_0 is large many different modes contribute to the entropy. To get an accurate result for a system in which many modes are important requires using many oscillators, which is computationally intractable. Instead, we take the even wavenumber spacing of section 4.3.1 as given and derive a bound on the entropy from that ansatz.

5.1 The first outside oscillator

With the wavenumber spacing fixed we have one free parameter, the spacing k_1 , which depends on the energy E_0 . To fix k_1 we we examine the expectation value of $w_{N_{\text{in}}+1}^2$. Since this is an outside operator, it must have the same value in the vacuum as in a vacuum-bounded state. The vacuum value is straightforward to compute, and we show below that in the vacuum-bounded state the value depends only on the wavenumbers. In fact, we will be able to derive only an upper bound in the vacuum case and only a lower bound in the case of a vacuum-bounded state. However, these bounds are sufficient to derive a lower bound on k_1 and thus an upper bound on $S(E)$.

5.1.1 The vacuum

In section 3.2.8 we computed the values of $\langle \mathbb{X} \rangle$. To convert to \mathbf{w} coordinates we proceed as follows: From section 3.2.4, $\mathbf{x} = Q\mathbf{w}$ and so

$$\mathbf{x}_{\text{out}} = R\mathbf{w}_{\text{out}} = D\mathbf{w}_{\text{mid}} + Y_{\text{out,gs}}\mathbf{w}_{\text{gs}}. \quad (5.1)$$

In the numerical work we found that with our choice for D we got

$$\tilde{K}_{\text{in,mid}} = \begin{pmatrix} & 0 \\ -\bar{g} & \end{pmatrix}. \quad (5.2)$$

Since

$$\tilde{K}_{\text{in,mid}} = K_{\text{in,out}} D = \begin{pmatrix} & 0 \\ \overline{-g} & \end{pmatrix} D \quad (5.3)$$

it follows that the first row of D is $(1, 0 \dots 0)$. Thus from Eq. (5.1) we get

$$x_{N_{\text{in}}+1} = w_{N_{\text{in}}+1} + (Y_{\text{out,gs}})_1 \cdot \mathbf{w}_{\text{gs}} \quad (5.4)$$

where $(Y_{\text{out,gs}})_1$ denotes the first row of $Y_{\text{out,gs}}$. Now $\widetilde{\mathbb{W}}_{\text{gs,gs}} = (1/2)I$ and $\widetilde{\mathbb{W}}_{\text{gs,free}} = 0$, so

$$\langle x_{N_{\text{in}}+1}^2 \rangle = \langle w_{N_{\text{in}}+1}^2 \rangle + \frac{1}{2} (Y_{\text{gs,out}} Y_{\text{gs,out}}^T)_{11} . \quad (5.5)$$

Since the last term is non-negative, we have

$$\langle w_{N_{\text{in}}+1}^2 \rangle^{\text{vac}} \leq \langle x_{N_{\text{in}}+1}^2 \rangle^{\text{vac}} . \quad (5.6)$$

From Eq. (3.85) we have

$$\langle x_{N_{\text{in}}+1}^2 \rangle^{\text{vac}} = \langle \mathbb{X} \rangle_{N_{\text{in}}+1, N_{\text{in}}+1} = \frac{L_1}{2\pi} \left[\psi \left(2N_{\text{in}} + \frac{5}{2} \right) - \psi \left(\frac{1}{2} \right) \right] \quad (5.7)$$

We would like to evaluate this expression in the $N_{\text{in}} \rightarrow \infty$ limit with L_{in} fixed. There is a prefactor of L_1 , which goes to zero in this limit, but that is just an artifact of the conventions we have used for the discrete problem, and will appear in the finite-energy vacuum-bounded states as well. For large x ,

$$\psi(x) \sim \ln x + O(1/x) , \quad (5.8)$$

so without the prefactor there is a logarithmic divergence. We are interested in the $\ln N_{\text{in}}$ term, and in the constant term, but we will ignore any terms of order $1/N_{\text{in}}$ or lower.

We use Eq. (5.8) and $\psi(1/2) = -\gamma - 2 \ln 2$, where γ is Euler's constant, to get

$$\langle x_{N_{\text{in}}+1}^2 \rangle^{\text{vac}} = \frac{L_1}{2\pi} \left[\ln 2N_{\text{in}} + \gamma + 2 \ln 2 + O\left(\frac{1}{N_{\text{in}}}\right) \right] \quad (5.9)$$

and so

$$\langle w_{N_{\text{in}}+1}^2 \rangle^{\text{vac}} \leq \langle x_{N_{\text{in}}+1}^2 \rangle^{\text{vac}} = \frac{L_1}{2\pi} \left[\ln 8N_{\text{in}} + \gamma + O\left(\frac{1}{N_{\text{in}}}\right) \right] . \quad (5.10)$$

5.1.2 Evenly spaced wavenumbers

Now we will compute the same correlator in the vacuum-bounded system, using the ansatz that the wavenumbers are multiples of some spacing k_1 . From Eq. (3.100a) we have

$$\langle w_{N_{\text{in}}+1}^2 \rangle = \sum_{\alpha} \frac{1}{2\omega_{\alpha}} (w_{N_{\text{in}}+1}^{\alpha})^2 \coth \left(\frac{\beta}{2} \omega_{\alpha} \right) . \quad (5.11)$$

There are $N_{\text{norm}} \approx \pi/k_1$ normal modes which are sine waves in the inside region. These modes are equivalent to the modes that we would have for a problem with a rigid boundary at position

$$L'_{\text{in}} \equiv N_{\text{norm}} L_1 \approx \frac{\pi}{k_1} L_1. \quad (5.12)$$

There are also $N_{\text{free}} - N_{\text{norm}}$ abnormal modes. We do not know how to compute the contribution of the abnormal modes to the correlator. However, the contribution from each mode is positive, so by taking only normal modes we will find a lower bound on $\langle w_{N_{\text{in}}+1}^2 \rangle$.

From Eq. (3.108) for the normal modes we have

$$w_\mu^n = N_n \sin \mu k_n \quad (5.13)$$

for $\mu = 1 \dots N_{\text{in}} + 1$. Putting this in Eq. (5.11) we get

$$\begin{aligned} \langle w_{N_{\text{in}}+1}^2 \rangle &= \sum_{n=1}^{N_{\text{norm}}} \frac{1}{2\omega_n} \coth \left(\frac{\beta}{2} \omega_n \right) N_n^2 \sin^2 k_n (N_{\text{in}} + 1) + \text{abnormal modes} \\ &\geq \sum_{n=1}^{N_{\text{norm}}} \frac{1}{2\omega_n} \coth \left(\frac{\beta}{2} \omega_n \right) N_n^2 \sin^2 k_n (N_{\text{in}} + 1) \end{aligned} \quad (5.14)$$

since the abnormal mode contribution is positive.

The important point here is that we know w_μ^n for μ up to $N_{\text{in}} + 1$, and we know $\langle w_\mu w_\nu \rangle$ for μ and ν down to $N_{\text{in}} + 1$. Thus taking $\mu = \nu = N_{\text{in}} + 1$ gives the unique correlator for which we know the components that go into the expression for the correlator while also knowing that the correlator must have the same value as in the vacuum. The same argument does not work for $\langle P_{w_{N_{\text{in}}+1}} P_{w_{N_{\text{in}}+1}} \rangle$, because we know the inverse mode matrix only up to $\mu = N_{\text{in}}$ and not $\mu = N_{\text{in}} + 1$.

Now we will compute the right-hand side of Eq. (5.14) in the limit where N_{in} and N_{norm} are large. We will ignore all terms of $O(1/N_{\text{in}})$ or $O(1/N_{\text{norm}})$ and so take $L'_{\text{in}}/N_{\text{norm}} = L_{\text{in}}/N_{\text{in}}$. We use

$$k_n = n k_1 = \frac{\pi n}{N_{\text{norm}}} \quad (5.15)$$

and

$$\omega_n = \frac{2}{L_1} \sin \frac{k_n}{2} = \frac{2}{L_1} \sin \frac{\pi n}{2N_{\text{norm}}}. \quad (5.16)$$

First we must derive the normalizations of the normal modes. With our choice of normalization,

$$\sum_n w_\mu^n w_\nu^n = T'_{\mu\nu}. \quad (5.17)$$

Thus if a is an inside oscillator, then for any μ ,

$$\sum_n w_a^n w_\mu^n = \delta_{a\mu} \quad (5.18)$$

so

$$\delta_{a\mu} = \sum_{n=1}^{N_{\text{norm}}} N_n^2 \sin k_n a \sin k_n \mu + \text{abnormal modes}. \quad (5.19)$$

We would like to use Eq. (5.19) to determine the normalization factors N_n , but first we have to dispose of the abnormal mode term. Later we will find that N_{norm} is close to N_{in} . Using this, and since we are working in the limit where N_{in} is large, we can choose a such that

$$1 \ll a \ll 2N_{\text{in}} - N_{\text{norm}} \sim N_{\text{in}}. \quad (5.20)$$

Each abnormal mode n contributes

$$N_n^2 \sinh k_n a \sinh k_n \mu \equiv \delta_{\text{abn}}^{(n)} \quad (5.21)$$

to the right-hand side of Eq. (5.19). However, this same mode contributes

$$\frac{L_1}{4} N_n^2 \frac{\sinh^2 k_n (N_{\text{in}} + 1)}{\cosh(k_n/2)} \quad (5.22)$$

to the sum for $\langle w_{N_{\text{in}}+1}^2 \rangle$ in Eq. (5.14). Since $\langle w_{N_{\text{in}}+1}^2 \rangle \leq L_1/(2\pi)[\ln N_{\text{in}} + O(1)]$ it follows that

$$N_n^2 \frac{\sinh^2 k_n (N_{\text{in}} + 1)}{\cosh(k_n/2)} \lesssim \frac{2}{\pi} \ln N_{\text{in}} \quad (5.23)$$

for each n and thus that

$$\delta_{\text{abn}}^{(n)} < \frac{2 \sinh k_n a \sinh k_n \mu \cosh(k_n/2)}{\pi \sinh^2 k_n (N_{\text{in}} + 1)} \ln N_{\text{in}}. \quad (5.24)$$

The exact values of the k_n for the abnormal modes vary with N_{in} . For successive N_{in} values, each k_n decreases toward 0 until the corresponding mode converts to a normal mode as described in section 4.3. By avoiding the points where these “conversions” are about to take place it is possible to find a sequence of values for N_{in} which have all $k_n \gtrsim 1$. For such values,

$$\delta_{\text{abn}}^{(n)} \lesssim e^{-k_n(2N_{\text{in}}-a-\mu+3/2)}. \quad (5.25)$$

From Eq. (5.20) the exponent in Eq. (5.25) is $\ll -1$, so $\delta_{\text{abn}}^{(n)}$ is exponentially small. Since there are at most N_{in} abnormal modes, their total contribution to (5.19) is exponentially suppressed.

Thus we ignore the abnormal modes in Eq. (5.19), multiply by $\sin k_m \mu$ and sum

over μ to get

$$\begin{aligned}
\sin k_m a &= \sum_{\mu=1}^{N_{\text{norm}}} \sin k_m \mu \sum_{n=1}^{N_{\text{norm}}} N_n^2 \sin k_n a \sin k_n \mu \\
&= \sum_{n=1}^{N_{\text{norm}}} N_n^2 \sin k_n a \sum_{\mu=1}^{N_{\text{norm}}} \sin \frac{\pi m \mu}{N_{\text{norm}}} \sin \frac{\pi n \mu}{N_{\text{norm}}} \\
&= \sum_{n=1}^{N_{\text{norm}}} N_n^2 \sin k_n a \cdot \frac{N_{\text{norm}}}{2} \delta_{mn} \\
&= N_m^2 \frac{N_{\text{norm}}}{2} \sin k_m a,
\end{aligned} \tag{5.26}$$

from which we conclude that

$$N_m^2 = \frac{2}{N_{\text{norm}}} \tag{5.27}$$

for each mode m . Putting this in Eq. (5.14) gives

$$\langle w_{N_{\text{in}}+1}^2 \rangle \gtrsim \sum_{n=1}^{N_{\text{norm}}} \frac{\sin^2 k_n (N_{\text{in}} + 1)}{N_{\text{norm}} \omega_n} \coth \left(\frac{\beta}{2} \omega_n \right). \tag{5.28}$$

Note that Eq. (5.28) does not depend on N but only N_{norm} .

Let us define a dimensionless parameterization of the departure from the vacuum state,

$$\Delta = \frac{N_{\text{norm}} - N_{\text{in}}}{N_{\text{norm}}} \approx \frac{L'_{\text{in}} - L_{\text{in}}}{L'_{\text{in}}} \tag{5.29a}$$

$$\tau' = L'_{\text{in}} T = L'_{\text{in}} / \beta. \tag{5.29b}$$

Then $\sin^2 k_n (N_{\text{in}} + 1) = \sin^2 n\pi (1 - \Delta) = \sin^2 n\pi \Delta$. With ω_n from Eq. (5.16) we get

$$\langle w_{N_{\text{in}}+1}^2 \rangle \gtrsim \frac{L_1}{2} \sum_{n=1}^{N_{\text{norm}}} \frac{\sin^2 n\pi \Delta}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}} \coth \left(\frac{\beta}{L_1} \sin \frac{n\pi}{2N_{\text{norm}}} \right). \tag{5.30}$$

In the limit of large N_{free} , the argument of \coth becomes $\beta\pi n / (2L_1 N_{\text{norm}}) \approx \pi n / (2\tau')$. We expand $\coth x = 1 + 2/(e^{2x} - 1)$ to get

$$\langle w_{N_{\text{in}}+1}^2 \rangle \gtrsim \frac{L_1}{2} \sum_{n=1}^{N_{\text{norm}}} \frac{\sin^2 n\pi \Delta}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}} \left(1 + \frac{2}{(e^{-\pi n/\tau'} - 1)} \right). \tag{5.31}$$

We work first with the term not involving τ' . We expand the numerator using $\sin^2 x =$

$(1 - \cos 2x)/2$ to get

$$\frac{L_1}{4} \sum_{n=1}^{N_{\text{norm}}} \left(\frac{1}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}} - \frac{\cos 2n\pi\Delta}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}} \right). \quad (5.32)$$

This first term is the one that diverges as $N_{\text{norm}} \rightarrow \infty$. We can separate out the divergent part to get

$$\frac{L_1}{2\pi} \sum_{n=1}^{N_{\text{norm}}} \frac{1}{n} + \frac{L_1}{4} \sum_{n=1}^{N_{\text{norm}}} \left(\frac{1}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}} - \frac{2}{\pi n} \right). \quad (5.33)$$

The first term of Eq. (5.33) gives

$$\frac{L_1}{2\pi} (\ln N_{\text{norm}} + \gamma). \quad (5.34)$$

The second term of Eq. (5.33) is finite and can be converted to an integral in the $N_{\text{norm}} \rightarrow \infty$ limit, to give

$$\frac{L_1}{4} \int_0^1 dx \left(\frac{1}{\sin \frac{\pi x}{2}} - \frac{2}{\pi x} \right) = \frac{L_1}{2\pi} \left[\ln \left(\frac{1}{x} \tan \frac{\pi x}{4} \right) \right]_0^1 = \frac{L_1}{2\pi} \ln \frac{4}{\pi}. \quad (5.35)$$

The remaining term of Eq. (5.32) is

$$-\frac{L_1}{4} \sum_{n=1}^{N_{\text{norm}}} \frac{\cos 2n\pi\Delta}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}}. \quad (5.36)$$

To compute this we use $1/\sin x = \csc x = 1/x + x/6 + 7x^3/360 + \dots$ to get

$$-\frac{L_1}{4} \sum_{n=1}^{N_{\text{norm}}} \left(\frac{2}{\pi n} + \frac{\pi}{12} \frac{n}{N_{\text{norm}}^2} + \frac{7\pi}{2880} \frac{n^3}{N_{\text{norm}}^4} + \dots \right) \cos 2n\pi\Delta. \quad (5.37)$$

The first term can be summed in the $N_{\text{norm}} \rightarrow \infty$ limit,

$$-\frac{1}{2\pi} \sum_1^\infty \frac{\cos 2n\pi\Delta}{n} = \frac{1}{2\pi} \ln (2 \sin \pi\Delta). \quad (5.38)$$

The rest of the terms do not contribute. Because of the oscillations of the cosine, $\sum_1^{N_{\text{norm}}} n^k \cos n\pi\Delta$ goes as N_{norm}^k rather than N_{norm}^{k+1} and thus is killed by the corresponding N_{norm}^{k+1} in the denominator.

Putting Eqs. (5.34), (5.35) and (5.38) together, the first term on the right of Eq. (5.31) gives

$$\frac{L_1}{2\pi} \left(\ln \frac{8N_{\text{norm}} \sin \pi\Delta}{\pi} + \gamma \right). \quad (5.39)$$

We now look at the second term of Eq. (5.31),

$$L_1 \sum_{n=1}^{N_{\text{norm}}} \frac{\sin^2 n\pi\Delta}{N_{\text{norm}} \sin \frac{n\pi}{2N_{\text{norm}}}} \frac{1}{(e^{-\pi n/\tau'} - 1)}. \quad (5.40)$$

Here the divergence is cut off by the exponential in the denominator. We again expand using $1/\sin x = 1/x + x/6 + \dots$. The first term has no N_{norm} dependence and we can extend the sum to ∞ . In the next term, the sum is cut off by the exponential in the denominator, leading to a term of order $(\tau'/N_{\text{norm}})^2$. Further terms have higher powers of τ'/N_{norm} . In the limit $N_{\text{norm}} \rightarrow \infty$ we ignore all these terms, which leaves

$$\frac{2L_1}{\pi} \sum_{n=1}^{\infty} \frac{\sin^2 n\pi\Delta}{n (e^{\pi n/\tau'} - 1)}. \quad (5.41)$$

We are interested in the high-energy limit, for which $\tau' \gg 1$. Later we will see that Δ is of order $\ln \tau'/\tau' \ll 1$. Thus the summand in Eq. (5.41) is slowly varying and we can convert the sum into an integral,

$$\frac{2L_1}{\pi} \int_0^{\infty} \frac{\sin^2 \pi\Delta x \, dx}{x (e^{\pi x/\tau'} - 1)}. \quad (5.42)$$

The error in Eq. (5.42) is approximately the term that we would have for $n \rightarrow 0$ in Eq. (5.41). Taking this limit we find that the error has order $\Delta^2 \tau' \sim (\ln \tau')^2/\tau' \ll 1$, so our approximation is good. The integral in Eq. (5.42) can be done and the result is

$$L_1 \tau' \Delta + \frac{L_1}{2\pi} \ln \frac{1 - e^{-4\pi\tau'\Delta}}{4\pi\tau'\Delta}. \quad (5.43)$$

Putting together Eqs. (5.39) and (5.43) we find

$$\langle w_{N_{\text{in}}+1}^2 \rangle \gtrsim \frac{L_1}{2\pi} \left(\ln \frac{8N_{\text{norm}} \sin \pi\Delta}{\pi} + \gamma + 2\pi\tau' \Delta + \ln \frac{1 - e^{-4\pi\tau'\Delta}}{4\pi\tau'\Delta} \right). \quad (5.44)$$

Now we set $\langle w_{N_{\text{in}}+1}^2 \rangle = \langle w_{N_{\text{in}}+1}^2 \rangle^{\text{vac}}$ from Eq. (5.10) to get

$$\ln \frac{8N_{\text{in}}}{\pi} \gtrsim \ln \frac{8N_{\text{norm}} \sin \pi\Delta}{\pi} + 2\pi\tau' \Delta + \ln \frac{1 - e^{-4\pi\tau'\Delta}}{4\pi\tau'\Delta} \quad (5.45)$$

or

$$2\pi\tau' \Delta + \ln \frac{1 - e^{-4\pi\tau'\Delta}}{4\pi\tau'\Delta} \lesssim \ln \frac{N_{\text{in}}}{N_{\text{norm}} \sin \pi\Delta}. \quad (5.46)$$

Now we use $N_{\text{in}}/N_{\text{norm}} = 1 - \Delta$ from Eq. (5.29a) and approximate $\sin \pi\Delta \approx \pi\Delta$ since Δ is small. Since this is already $O(\Delta)$ we then approximate $(1 - \Delta)/\Delta \approx 1/\Delta$ to get

$$2\pi\tau' \Delta + \ln \frac{1 - e^{-4\pi\tau'\Delta}}{4\pi\tau'\Delta} \lesssim \ln \frac{1}{\pi\Delta}. \quad (5.47)$$

Thus $\Delta \leq \Delta_{\max}$ where

$$\Delta_{\max} = \frac{1}{2\pi\tau'} \ln \frac{4\tau'}{1 - e^{-4\pi\tau'\Delta_{\max}}}. \quad (5.48)$$

If instead of $\tau' = L'_{\text{in}}T$ we use

$$\tau \equiv L_{\text{in}}T \quad (5.49)$$

we will make an error of order Δ_{\max} , which we expect to be small. We ignore this second order contribution and take τ' as τ in Eq. (5.48),

$$\Delta_{\max} = \frac{1}{2\pi\tau} \ln \frac{4\tau}{1 - e^{-4\pi\tau\Delta_{\max}}}. \quad (5.50)$$

If we ignore $e^{-4\pi\tau\Delta_{\max}}$ in the denominator we get

$$\Delta_{\max} = \frac{1}{2\pi\tau} \ln 4\tau. \quad (5.51)$$

Using this we find that $e^{-4\pi\tau\Delta_{\max}} = (4\tau)^{-2} \ll 1$ since $\tau \gg 1$, which justifies ignoring this term. We will also ignore $\ln 4$ by comparison with $\ln \tau$. Thus we conclude

$$\Delta \lesssim \frac{1}{2\pi\tau} \ln \tau + O\left(\frac{1}{\tau}\right) = \frac{1}{2\pi L_{\text{in}}T} \ln L_{\text{in}}T + O\left(\frac{1}{L_{\text{in}}T}\right) \quad (5.52)$$

and

$$L'_{\text{in}} \leq L_{\text{in}} + \frac{1}{2\pi T} \ln L_{\text{in}}T + O\left(\frac{1}{T}\right). \quad (5.53)$$

The equivalent system is larger by at most a thermal wavelength times a logarithmic factor depending on the inside size.

5.2 Propagation of bounds

In the previous section we derived an expression that gives the frequencies, and thus the entropy, for a vacuum-bounded system at a given temperature $T = 1/\beta$. Given such an expression, we would like to compute the entropy as a function of energy. Unfortunately the energy is not simple to compute from the frequencies alone.¹ However, we can easily compare the entropy of the vacuum-bounded system to that of a system with a rigid boundary at L_{in} and the same temperature. To make this comparison at fixed energy instead, we proceed as follows.

¹Such a computation can be done, but since E needs to be renormalized against the ground-state energy of the entire system, the result depends sensitively on the frequencies and normalizations even for very high-energy modes.

Consider the free energy $F = E - TS$ which has $dF = -SdT$. Integrating gives

$$E - TS = - \int_0^T S(T')dT'. \quad (5.54)$$

Let S^{rb} and T^{rb} denote the entropy and temperature of the system with a rigid boundary at L_{in} , and S and T denote those for the vacuum bounded system. For any quantity A let $\delta A(T)$ denote the difference between vacuum-bounded and rigid box systems at fixed temperature, $\delta A(T) \equiv A(T) - A^{\text{rb}}(T)$, and $\delta A(E)$ denote the same difference at fixed energy, $\delta A(E) \equiv A(E) - A^{\text{rb}}(E)$. With E fixed we compare the differences (to first order) in the two sides of Eq. (5.54) between the vacuum-bounded and rigid box systems,

$$-T\delta S(E) - \delta T(E)S = -\delta T(E)S - \int_0^T \delta S(T')dT', \quad (5.55)$$

where the first term on the right-hand side comes from the change in the integration limit. Thus

$$\delta S(E) = \frac{1}{T} \int_0^T \delta S(T')dT'. \quad (5.56)$$

5.3 The final entropy bound

Now we apply Eq. (5.56) to the case of section 5.1 where

$$\omega_n \approx \frac{n\pi}{L'_{\text{in}}} \quad \text{and} \quad L'_{\text{in}} \approx L_{\text{in}}(1 + \Delta) \quad (5.57)$$

with

$$\Delta L_{\text{in}} \leq \frac{1}{2\pi T} \ln L_{\text{in}} T. \quad (5.58)$$

At any given temperature, the vacuum-bounded system has the entropy $S(T)$ of a system of length L'_{in} . Now in a one-dimensional system the entropy density is proportional to the temperature,

$$S^{\text{rb}} = \frac{\pi}{3} L_{\text{in}} T, \quad (5.59)$$

and thus the entropy difference between vacuum-bounded and rigid box systems is

$$\delta S(T) = \frac{\pi}{3} \Delta L_{\text{in}} T \leq \frac{1}{6} \ln L_{\text{in}} T. \quad (5.60)$$

Using Eq. (5.56) we get²

$$\delta S(E) \leq \frac{1}{T} \int_0^T \frac{1}{6} \ln L_{\text{in}} T' dT' = \frac{1}{6} (\ln L_{\text{in}} T - 1) . \quad (5.61)$$

Since we are ignoring terms of order 1 by comparison with those of order $\ln T$, we can write

$$\delta S(E) \lesssim \frac{1}{6} \ln L_{\text{in}} T \approx \frac{1}{6} \ln S^{\text{rb}} . \quad (5.62)$$

Thus we conclude that the vacuum-bounded condition closely approximates the rigid box of length L_{in} . For the same energy, the vacuum-bounded condition allows slightly more entropy. The entropy difference grows at most logarithmically with rigid box entropy. For high energies, $S^{\text{rb}} \gg 1$ so we conclude that $\delta S \ll S^{\text{rb}}$.

5.4 Discussion

We have introduced a new way of specifying that matter and energy are confined to a particular region of space. Rather than giving a boundary condition per se, we specify a condition on a density matrix describing the state of the overall system. We require that any measurement which does not look into the inside region cannot distinguish our system from the vacuum. This avoids certain difficulties such as the Casimir energy that results from the introduction of a boundary and the geometric entropy [31,32] that results from ignoring part of a system. For these *vacuum-bounded* states, we consider the problem of finding the maximum-entropy state for a given total energy. This is analogous to the problem of finding the thermal state in a system with a rigid boundary.

Unfortunately, the vacuum-bounded problem is more difficult than the analogous problem with a rigid boundary and we must resort to working in one dimension and to numerical solution on a lattice. It is, however, possible to reduce the problem to a finite number of degrees of freedom, even when the outside region is infinitely large. From the numerical solution we justify the ansatz that the continuum wavenumbers are evenly spaced in this problem. Using this ansatz we compute an upper bound on the entropy of a vacuum-bounded state, and show that for high energies ($ER \gg 1$) the entropy approaches that of a system with rigid boundaries. Of course this is what one would expect for a system whose typical wavelengths are much shorter than the size of the inside region.

To apply this result to an evaporating black hole we look at the state produced by the black hole after evaporation [5]. Since our calculation was one-dimensional we must assume that the similarity between the vacuum-bounded state and the thermal state with a rigid boundary extends to three dimensions. Then we infer that very

²It happens that $\delta S(E)$ and $\delta S(T)$ are approximately the same, but that is a particular property of the system at hand. For example, if Δ were a constant we would have $\delta S(E) = 1/T \int_0^T c \Delta L_{\text{in}} T' dT' = 2c \Delta L_{\text{in}} T = 2\delta S(T)$.

little entropy can be emitted in the final explosion, in accord with the results of Aharonov, Casher and Nussinov [24] and Preskill [5]. For example, a black hole formed in the big bang with mass of order $10^{15}g$ would be evaporating today. During its life it would have radiated entropy $S \sim 10^{38}$. Now we assume that the entropy of the final explosion has energy $E \sim 10^{19}\text{erg}$ contained in radius $R \sim 10^{-23}\text{cm}$ as in section 1.2.1, and that the maximum entropy is not too different from that of a spherical box, in accord with our one-dimensional result. Then we find that the final explosion can emit only entropy $S \sim 10^{10}$, which is a factor of 10^{28} less than what was emitted earlier in the thermal radiation. The choice of T_{unk} is somewhat arbitrary, but whatever value one chooses there is some fixed bound on the emission of entropy after T_{unk} is reached. By considering a sufficiently large starting black hole, and thus sufficient entropy emission at early times, one always finds that the late time information is too little to produce a final pure state.

This argument means that a black hole must not evaporate completely but rather leave a remnant or remnants, that information must be lost, or else that the Hawking radiation is not exactly thermal, even at very early times [16].

Appendix

Low Energy Results

In the low-energy regime we do not see the linear wavenumber relation that we see in the high-energy case (Fig. 4-9). Instead, for sufficiently low temperature, the wavenumbers and frequencies are nearly the same as in the reduced vacuum. These frequencies are much lower than in a rigid box with the same L_{in} . At low temperatures, the entropy depends only on the low-lying frequencies and on β . Thus we expect that there will be significantly more entropy in a vacuum-bounded state than a rigid box state of the same energy. While we don't know how to construct an analytic proof of this claim, we will outline a general argument here, and make a conjecture supported by numerical data.

In the low-energy regime we can make a first-order expansion around the vacuum. To do this we note that the only dependence on β in our equations is through $\coth(\beta\omega_\alpha/2)$ in Eqs. (3.100). For large β we can approximate

$$\coth \frac{\beta\omega_\alpha}{2} \approx 1 + 2e^{-\beta\omega_\alpha}. \quad (\text{A.1})$$

The change in $\coth(\beta\omega_\alpha/2)$ is the largest for the smallest frequency, which we will call ω_1 . We will ignore $e^{-\beta\omega_\alpha}$ for larger ω_α by comparison with $e^{-\beta\omega_1}$. Thus we take

$$\delta \coth \frac{\beta\omega_1}{2} = 2e^{-\beta\omega_1^{\text{vac}}} \equiv 2\epsilon \quad (\text{A.2a})$$

$$\delta \coth \frac{\beta\omega_\alpha}{2} = 0 \quad \text{for } \alpha > 1. \quad (\text{A.2b})$$

Then we write

$$T'_{\text{mid,mid}} = \tilde{T}_{\text{mid,mid}} + \delta T_{\text{mid,mid}} \quad (\text{A.3a})$$

$$K'_{\text{mid,mid}} = \tilde{K}_{\text{mid,mid}} + \delta K_{\text{mid,mid}} \quad (\text{A.3b})$$

where $\delta K_{\text{mid,mid}}$ and $\delta T_{\text{mid,mid}}$ are $O(\epsilon)$. These changes give rise to $O(\epsilon)$ changes in U and the ω_α , which in turn give rise to $O(\epsilon)$ changes in $\langle w_m w_n \rangle$ and $\langle P_{w_m} P_{w_n} \rangle$.

Since overall $\langle w_m w_n \rangle$ and $\langle P_{w_m} P_{w_n} \rangle$ cannot change we must have

$$0 = \delta \langle w_m w_n \rangle = \sum_{\alpha} \left(-\frac{\delta \omega_{\alpha}}{2\omega_{\alpha}^2} U_{m\alpha}^{\text{vac}} U_{n\alpha}^{\text{vac}} + \frac{1}{2\omega_{\alpha}^{\text{vac}}} \delta U_{m\alpha} U_{n\alpha}^{\text{vac}} + \frac{1}{2\omega_{\alpha}^{\text{vac}}} U_{m\alpha} \delta U_{n\alpha} \right) + \frac{1}{\omega_1^{\text{vac}}} U_{m1}^{\text{vac}} U_{n1}^{\text{vac}} \epsilon \quad (\text{A.4a})$$

$$0 = \delta \langle P_{w_m} P_{w_n} \rangle = \sum_{\alpha} \left(\frac{\delta \omega_{\alpha}}{2} U_{\alpha m}^{\text{vac}} U_{\alpha n}^{\text{vac}} + \frac{\omega_{\alpha}^{\text{vac}}}{2} \delta U_{\alpha m}^{-1} U_{\alpha n}^{\text{vac}} + \frac{\omega_{\alpha}^{\text{vac}}}{2} U_{\alpha m}^{\text{vac}} U_{\alpha n}^{-1} \right) + \omega_1^{\text{vac}} U_{m1}^{\text{vac}} U_{n1}^{\text{vac}} \epsilon. \quad (\text{A.4b})$$

We thus have $N_{\text{in}}(N_{\text{in}} + 1)$ linear equations for $N_{\text{in}}(N_{\text{in}} + 1)$ unknown values of $\delta T_{\text{mid},\text{mid}}$ and $\delta K_{\text{mid},\text{mid}}$, which are readily solved. Since the inhomogeneous part of these equations is $O(\epsilon)$, all the results must be $O(\epsilon)$ as well. In particular, the $\delta \omega_{\alpha}$ are $O(\epsilon)$. Now if T is very small as compared to all the ω_{α} , then ϵ will be small as compared to all the parameters of the problem, and so the first-order approximation will be good. For any fixed number of oscillators N_{in} there will be some minimum frequency ω_1 , and if we take $\beta \ll 1/\omega_1$ we will always be in this regime.

Now the entropy S depends only on β and the ω_{α} . Since the modes are uncoupled,

$$S = \sum_{\alpha} S_1(\beta \omega_{\alpha}) \quad (\text{A.5})$$

with

$$S_1(\beta \omega) = -\ln(1 - e^{-\beta \omega}) + \frac{\beta \omega}{e^{-\beta \omega} - 1}. \quad (\text{A.6})$$

Since $\beta \omega_{\alpha} \gg 1$ all the terms are very small, and the ω_1 term dominates,

$$S \approx S_1(\omega_1) = (1 + \beta \omega_1) e^{-\beta \omega_1} + O(e^{-2\beta \omega_1}). \quad (\text{A.7})$$

Since ϵ drops exponentially with increasing β , we expect that for β large enough, $\beta \delta \omega_1 \ll 1$ so that

$$S = (1 + \beta \omega_1^{\text{vac}}) e^{-\beta \omega_1^{\text{vac}}} + O(\epsilon^2). \quad (\text{A.8})$$

The value of S given in Eq. (A.8) is the one we would get from a rigid box with length

$$L'_{\text{in}} = \pi / \omega_1^{\text{vac}}. \quad (\text{A.9})$$

To approximate the energy, we proceed along the lines of section 5.2. The direct calculation is made difficult by the fact that, while H' differs from H only by $O(\epsilon)$, we must subtract from both Hamiltonians a large ground-state energy. Instead we work by integrating on T . From Eq. (5.54) we have

$$E(T) = TS(T) - \int_0^T S(T') dT'. \quad (\text{A.10})$$

Now L'_{in} depends only on ω_1^{vac} , which depends on N_{in} but not on β . If Eq. (A.8) is valid for a particular N_{in} at $\beta = 1/T$ is it valid for $T' < T$ and $\beta' = 1/T' > \beta$. Thus

both $S(T)$ and $S(T')$ in Eq. (A.10) are just the entropy of a rigid box of length L'_{in} . Thus the entropy-to-energy relationship is just $S(E) = S^{\text{rb}}(L'_{\text{in}}; E)$, the entropy as a function of the given energy in a rigid box with length L'_{in} .

For such a rigid box at very low energy we find

$$E = \frac{\omega_1^{\text{rb}}}{e^{\beta\omega_1^{\text{rb}}} - 1} \approx \omega_1^{\text{rb}} e^{-\beta\omega_1^{\text{rb}}} \quad (\text{A.11})$$

and thus

$$S = \left(1 + \ln \frac{\omega_1^{\text{rb}}}{E}\right) \frac{E}{\omega_1^{\text{rb}}} \quad (\text{A.12})$$

where $\omega_1^{\text{rb}} = \pi/L'_{\text{in}} = \omega_1^{\text{vac}}$ is the frequency of the lowest mode.

Now for any given N_{in} we get some ω_1^{vac} . As discussed in section 4.2, the larger N_{in} we choose, the smaller ω_1^{vac} we will have. For N_{in} fixed we can choose $\beta \gg 1/\omega_1^{\text{vac}}$ and proceed as above to get a large value of L'_{in} . However, we are really interested in the continuum limit at fixed temperature. If we increase N_{in} with β fixed we will find that ω_1 (and eventually an arbitrary number of the ω_α) will become smaller than $1/\beta$. When this happens, the approximations of Eqs. (A.2–A.4) will no longer be good.

However, we do not expect the entropy to decrease drastically in this limit. To make the entropy small would require making all the frequencies large. If the frequencies were large, the approximations we have used would again become valid. Then we could argue as before that the entropy should be large. It would be hard to have a consistent picture.

Now consider the limit as $T \rightarrow 0$. For each T we start with some initial number of oscillators $N_{\text{in}}^{(0)}$. We choose $N_{\text{in}}^{(0)}$ not too large, such that $\omega_1^{\text{vac}} \gg T$. With this value of N_{in} , we find $L'_{\text{in}}^{(0)} \sim \pi/\omega_1^{\text{vac}}$. We then let $N_{\text{in}} \rightarrow \infty$ and we conjecture that the entropy does not change much, and thus in the continuum limit $S(E) \sim S^{\text{rb}}(L'_{\text{in}}^{(0)}; E)$. As we decrease T we can decrease the initial ω_1^{vac} and so increase $L'_{\text{in}}^{(0)}$ without bound. Thus we make the following conjecture:

For a given energy E , let $L'_{\text{in}}(E)$ be the length of a rigid box such that the vacuum-bounded state with energy E and length L'_{in} has entropy $S(E) = S^{\text{rb}}(L'_{\text{in}}(E); E)$. Then

$$\lim_{E \rightarrow 0} \frac{L'_{\text{in}}(E)}{L_{\text{in}}} = \infty. \quad (\text{A.13})$$

To support this conjecture numerically we turn to direct calculation of energy and entropy values for vacuum-bounded states at low temperature. For various fixed values of $\beta = 1/T$ and for various numbers of oscillators we compute S and E and from them the equivalent length L'_{in} . The results are plotted in Fig. A-1. While N_{in} is still small enough for the approximations Eqs. (A.2–A.4) to be valid, L'_{in} grows with N_{in} . Once N_{in} has left this regime, it appears that L'_{in} levels off. It is at least reasonable to believe that there is no further change in L'_{in} as $N_{\text{in}} \rightarrow \infty$. In Fig. A-2 we plot the eventual level of L'_{in} versus β . It appears that the limiting value of L'_{in} grows nearly linearly with β , and thus $L'_{\text{in}} \rightarrow \infty$ as $E \rightarrow 0$ as conjectured.

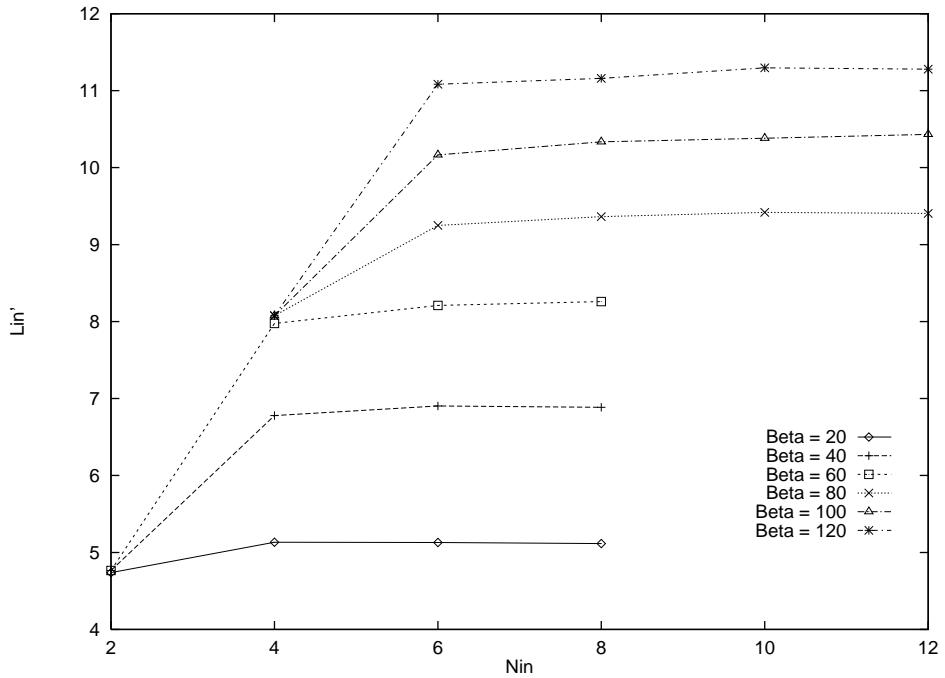


Figure A-1: The length L'_{in} of a rigid box that gives the same $S(E)$ as a vacuum-bounded state at temperature $T = 1/\beta$ and $L_{in} = 1.0$.

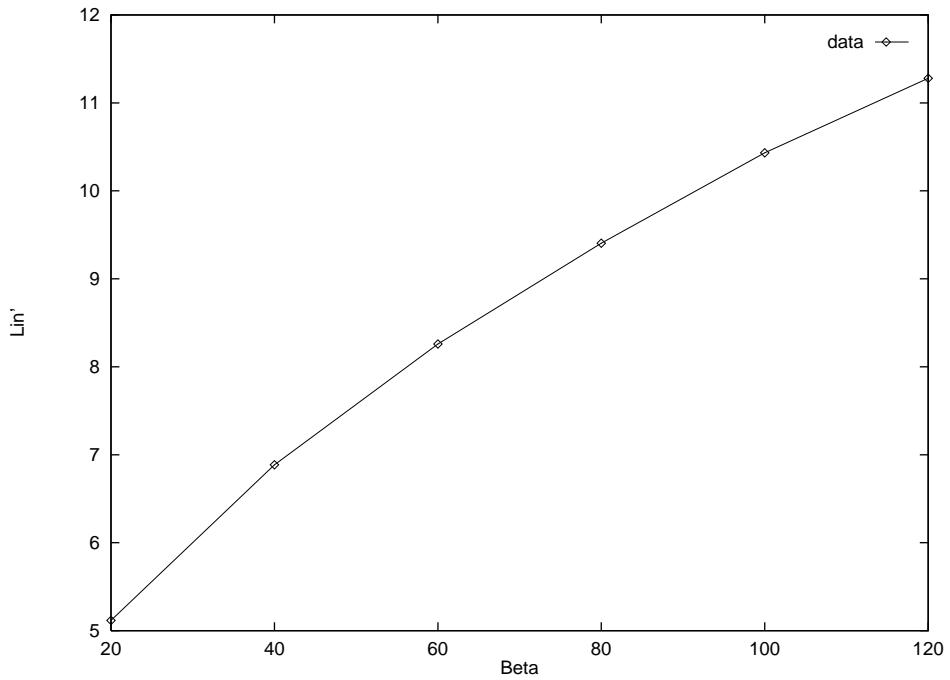


Figure A-2: The length L'_{in} of a rigid box with the same $S(E)$ plotted against β . Each point is the value for the largest number of oscillators available.

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